

# Mappings of open quantum systems onto chain representations and Markovian embeddings

M.P. Woods<sup>1,2</sup>, R. Groux<sup>3</sup>, A.W. Chin<sup>1</sup>, S.F. Huelga<sup>1</sup>, and M.B. Plenio<sup>1,2</sup>

<sup>1</sup> Institute für Theoretische Physik, Universität Ulm, D-89069 Ulm, Germany

<sup>2</sup> QOLS, Blackett Laboratory, Imperial College London, SW7 2BW, United Kingdom

<sup>3</sup> Lycée Polyvalent Rouvière, Rue Sainte Claire Deville. BP 1205, 83070 Toulon, France  
e-mail: mischa.woods05@imperial.ac.uk, roland.groux@orange.fr, alex.chin@uni-ulm.de, susana.huelga@uni-ulm.de, martin.plenio@uni-ulm.de

Received: date / Accepted: date

**Abstract** We derive a sequence of measures whose corresponding Jacobi matrices have special properties and a general mapping of an open quantum system onto 1D semi infinite chains with only nearest neighbour interactions. Then we proceed to use the sequence of measures and the properties of the Jacobi matrices to derive an expression for the spectral density describing the open quantum system when an increasing number of degrees of freedom in the environment have been embedded into the system. Finally, we derive convergence theorems for these residual spectral densities.

## 1 Introduction

### 1.1 Background

Real quantum mechanical systems are never found in complete isolation, but invariably coupled to a macroscopically large number of "environmental" degrees of freedom, such as those provided by electromagnetic field modes, density fluctuations of the surrounding media (phonons) or ensembles of other quantum systems, like electronic or nuclear spins [1,2,3]. The fact that the environment is totally or partially inaccessible to experimental probing in these so called "open quantum systems" leads to the appearance of an effectively irreversible dynamics for the quantum system's observables, and mediate the fundamental processes of energy relaxation, phase decoherence and, possibly, the thermalization of the subsystem.

Accurate numerical or analytical description of general open quantum systems dynamics appears, *prima facie*, to be extremely difficult due to the large (often infinite) number of bath and system variables which need to be accounted for. When the environmental degrees of freedom are modeled as a *bath* of harmonic oscillators exact path integral solutions can be available but are rarely of practical use [10,1,2]. Hence assumptions such as weak

system-environment coupling and vanishing correlation times of the environment, i.e. the Born-Markov approximation, are often invoked to obtain compact and efficiently solvable equations. These approaches suffer the drawback that their accuracy is hard to certify and that they become simply incorrect in many important situations. Indeed, our increasing ability to observe and control quantum systems on ever shorter time and length scales is constantly revealing new roles of noise and quantum coherence in important biological and chemical processes [4,5,6,7,8] and requires an accurate but efficient description of the system-environment interaction that go well beyond the Born-Markov approximation [8,9] in order to understand the interaction of intrinsic quantum dynamics and environmental noise. In many biological, chemical and solid-state systems, deviations from strict Markovianity, which can be explicitly quantified [11,12,13], are significant and methods beyond standard perturbative expansions are required for their efficient description. A number of techniques have been developed to operate in this regime. Those include polaron approaches [14], the quasi-adiabatic path-integral (QUAPI) method [15], the hierarchical equation of motion approach [16] and extensions of the quantum state diffusion description to non-Markovian regimes [17].

Here we will focus on the exploration of the mathematics of an exact, analytical mapping of the standard model of a quantum system interacting with a continuum of harmonic oscillators to an equivalent model in which the system couples to one end of a chain nearest-neighbour coupled harmonic oscillators, as illustrated in (a) of Fig. (1) and (b) of Fig. (1). This mapping has permitted the formulation of an efficient algorithm for the description of the system-environment coupling for arbitrary spectral densities of the environment fluctuations [18,19]. This new mapping which originally intended just as a practical means of implementing t-DMRG which would avoid approximate determination of the chain representation using purely numerical, and often unstable, transforms [20], it was quickly realised that the scope of the mapping is much broader. Indeed, the mapping itself provides an extremely intuitive and powerful way of analysing universal properties of open quantum systems, that is, independent of the numerical method used to simulate the dynamics [18]. This conclusion was implied also in [21], where the authors also developed a, in principle, rather different chain representation of a harmonic environment using an iterative propagator technique [21].

Both of these theories establish chain representations as a novel and direct way of looking at how energy and correlations propagate into the environment in real time. In the chain picture the interactions cause excitations to propagate away from the system, allowing a natural, causal understanding of Markovian and non-Markovian dissipation in terms of the properties of the chain's couplings and frequencies. An intuitive account of the physics of chain representations, non-Markovian dynamics and irreversibility for the method in [19, 18] is given in [22], and an interpretation of chain parameters in terms of time-correlations for the method in [21] can be found in [23].

## 1.2 This communication

The main goals of this paper can be split into two groups. Firstly, we aim at developing a general framework for mapping the environment of an open quantum system onto semi infinite 1D chain representations with nearest neighbour interactions where the system only

couples to the first element in the chain. In these chain representations, there is a natural and systematic way to "embed" degrees of freedom of the environment into the system (by "embed", we mean to redefine what we call system and environment by including some of the environmental degrees of freedom in the system) (c) of figure (1). One can make a non-Markovian system-environment interaction more Markovian by embedding some degrees of freedom of the environment into the system, a technique already employed in certain situations in quantum optics [24] and that recently has been demonstrated in all generality [21]. What remains unclear however, is to quantify how efficient such procedures can be as well as determining the best way of performing the embedding. We will show that those issues can be efficiently addressed with the formalism presented in this manuscript.

This general formalism allows the comparison between different chain mappings. Thus the second aim is to develop a method for understanding how Markovian such embeddings are by finding explicit analytical formulas for the spectral densities of the embeddings corresponding to the different chain mappings. Furthermore, we also derive universal convergence theorems for the spectral densities corresponding to the embedded systems and give rigorous conditions for when these limiting cases are achieved. This paves the way for a system interacting with a complex environment to be recast by moving the boundary of the system and environment, so that the non-trivial parts of the environment are embedded in the new effective "system" and the homogeneous chain represents the new, and much simpler, "environment" - See (c) in figure (1) for a pictorial illustration. The advantage of this is that the residual part of the environment might be simple enough for some of the approximations mentioned in section 1.1 to be applied, enabling us to integrate out these modes and dramatically reduce the number of sites of the chain that have to be accounted for explicitly. In order to achieve this, we have to first develop new mathematical tools and theorems regarding secondary measures and Jacobi operators, greatly extending and developing the application of orthogonal polynomials that was used in the original chain mapping of [18]. These results might be useful also in other areas of mathematics and mathematical physics which are related to the theory of Jacobi operators such as the Toda lattice [25].

We show that this generalised chain mapping reduces to two known results mentioned in section 1.1 under special conditions. For the first known result [19,18], the general method developed in this paper gives analytical and non-iterative expressions for the spectral densities corresponding to the embeddings. For the other special case [21], we derive calculable conditions for when the spectral densities corresponding to the embedding converge, -an aspect not addressed in [21]. As seen in the examples, we apply this technique to derive exact solutions for the family of Spin-Boson models which will allow us to illustrate how the different embedding methods are related. In addition, the method developed here is also valid when the spectral density of the system-environment interaction has a gap in its support region. This is of practical interest as there are open quantum systems (such as photonic crystals [26]) that naturally exhibit such a spectral density and hence can only be mapped onto a chain using the method presented in this paper.

The contents of each section is as follows: Section 2 is concerned with deriving the necessary mathematical tools for the application to open quantum systems in the subsequent sections. We start by introducing some elementary results in the field of orthogonal polynomials in section 2.1 (this section also helps to introduce notation). In section 2.2 we focus on deriving a formula which makes explicit a sequence of secondary measures solely in terms of the initial measure and its orthogonal polynomials. We point out that although

authors such as Gautschi introduce the concept and definition of secondary measures, here we provide for the first time an analytical closed expression for them in terms of the initial measure and its orthogonal polynomials. This result will turn out to be a vital ingredient in the development of the subsequent chapters. Moreover, Gautschi states that the general solution we have found is unknown [27] p16-17. In section 2.3 we study the properties of the 3-term recursion coefficients of the orthogonal polynomials generated from their measures. We then define beta normalised measures which have more general and useful properties. The main result of this section is our new theorem regarding the Jacobi matrix. This new theorem will be used extensively in section 3. Section 3 is concerned with chain mappings for open quantum systems and embeddings of environmental degrees of freedom into the system. In section 3.1 we develop a general framework for mapping open quantum systems which are linearly coupled to an environment onto a representation where the environment is a semi-infinite chain with nearest neighbour couplings and define two special cases of particular interest, - the particle and phonon mappings. In section 3.2, we investigate the relation between this work and recent work by [21]. In order to do this we make extensive use of the relations developed in section 2. We show how their mapping is a special case of the work presented here and find analytical non iterative solutions to quantities such as the sequence of partial spectral densities. Section 3.3 is dedicated to deriving the formulas for the sequence of partial spectral densities for the particle case mapping. In section 3.4 we develop convergence theorems for the sequence of partial spectral densities. We show rigorously that the sequence converges under certain conditions and give the universal functions the spectral densities converge to for the particle and phonon cases. The conditions for which the sequences converge are stated in terms of the initial spectral density. In section 4 we give explicit analytic examples for the family of spectral densities of the Spin-Boson model for the particle and phonon mapping cases. The main new results of this article are theorems (12), (15), (16), (17), (18), (19), (23) and corollaries (8) and (7).

## 2 Secondary measures

### 2.1 Introduction to notation and basic tools

**Definition 1** *Let us consider a measure  $d\mu(x) = \bar{\mu}(x)dx$  with real support interval  $I$  beginning at  $a$  and ending at  $b$  which has finite moments:*

$$C_n(d\mu) = \int_a^b x^n d\mu(x) \quad n = 0, 1, 2, \dots, \quad (1)$$

*with  $\bar{\mu}(x) > 0$  over  $I$  such that  $C_0(d\mu) > 0$ .*

We note that throughout this article, unless stated otherwise lower and upper values  $a$  and  $b$  can be finite or infinite.

**Definition 2** *Let  $\mathbb{P}$  denote the space of real polynomials. Then, for any  $u(x)$  and  $v(x) \in \mathbb{P}$  we will define an inner product as*

$$\langle u, v \rangle_{\bar{\mu}} = \int_a^b u(x)v(x)d\mu(x). \quad (2)$$

**Definition 3** We call  $\{P_n(d\mu; x)\}_{n=0}^{\infty}$  the set of real orthonormal polynomials with respect to measure  $d\mu$  where each polynomial  $P_n$  is of degree  $n$ , if they satisfy

$$\langle P_n(d\mu), P_m(d\mu) \rangle_{\bar{\mu}} = \delta_{nm} \quad n, m = 0, 1, 2, \dots \quad (3)$$

Similarly,

**Definition 4** We call  $\{\pi_n(d\mu; x)\}_{n=0}^{\infty}$  the set of real monic polynomials with respect to measure  $d\mu$  where each polynomial  $\pi_n$  is of degree  $n$  if they satisfy

$$\pi_n(d\mu; x) = P_n(d\mu; x)/a_n \quad n = 0, 1, 2, \dots, \quad (4)$$

where  $a_n = a_n(d\mu)$  is the leading coefficient of  $P_n(d\mu; x)$ .

**Theorem 1** For any measure  $d\mu(x)$ , there always exists a set of real orthonormal polynomials and real monic polynomials.

*Proof* See [27].

**Theorem 2** The monic polynomials  $\pi_n(d\mu; x)$  satisfy the three term recurrence relation

$$\pi_{n+1}(d\mu; x) = (x - \alpha_n)\pi_n(d\mu; x) - \beta_n\pi_{n-1}(d\mu; x) \quad n = 0, 1, 2, \dots, \quad (5)$$

$$\pi_{-1}(d\mu; x) := 0, \quad (6)$$

where

$$\alpha_n = \alpha_n(d\mu) = \frac{\langle x\pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}}{\langle \pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}} \quad n = 0, 1, 2, \dots, \quad (7)$$

$$\beta_n = \beta_n(d\mu) = \frac{\langle \pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}}{\langle \pi_{n-1}(d\mu), \pi_{n-1}(d\mu) \rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots \quad (8)$$

*Proof* See [27].

**Definition 5** We will define  $\beta_0(d\mu)$  by

$$\beta_0(d\mu) = \langle \pi_0(d\mu), \pi_0(d\mu) \rangle_{\bar{\mu}}. \quad (9)$$

**Corollary 1**  $\beta_0(d\mu) = C_0(d\mu)$ .

*Proof* We note that from definition (4),  $\pi_0(d\mu; x) = 1$  for all measures  $d\mu(x)$ . Hence,

$$\beta_0(d\mu) = \langle \pi_0(d\mu), \pi_0(d\mu) \rangle_{\bar{\mu}} = \int_a^b d\mu(x) = C_0(d\mu). \quad (10)$$

□

**Theorem 3** When the measure  $d\mu$  has bounded support, the  $\alpha_n(d\mu)$  and  $\beta_n(d\mu)$  coefficients are bounded by

$$a < \alpha_n(d\mu) < b \quad n = 0, 1, 2, \dots, \quad (11)$$

$$0 < \beta_n(d\mu) \leq \max(a^2, b^2) \quad n = 0, 1, 2, \dots \quad (12)$$

*Proof* See [27].

**Theorem 4** *The orthonormal polynomials  $P_n(d\mu; x)$  satisfy the three term recurrence relation*

$$t_n P_{n+1}(d\mu; x) = (x - s_n) P_n(d\mu; x) - t_{n-1} P_{n-1}(d\mu; x) \quad n = 0, 1, 2, \dots, \quad (13)$$

$$P_{-1}(d\mu; x) := 0, \quad P_0(d\mu; x) = 1/\sqrt{\beta_0(d\mu)}, \quad (14)$$

where

$$s_n = s_n(d\mu) = \alpha_n(d\mu) \quad n = 0, 1, 2, \dots, \quad (15)$$

$$t_n = t_n(d\mu) = \sqrt{\beta_{n+1}(d\mu)} \quad n = 0, 1, 2, \dots. \quad (16)$$

*Proof* See [27].

**Definition 6** *We will call  $Q_n(d\mu; x)$  the secondary polynomial<sup>1</sup> associated with polynomial  $P_n(d\mu; x)$  defined by*

$$Q_n(d\mu; x) = \int_a^b \frac{P_n(d\mu; t) - P_n(d\mu; x)}{t - x} d\mu(t), \quad n = 0, 1, 2, \dots \quad (17)$$

**Lemma 1** *The polynomials  $Q_n(d\mu; x)$ ,  $n = 1, 2, 3, \dots$  are real polynomials of degree  $n - 1$  and  $Q_0 = 0$ .*

*Proof* Follows from writing  $P_n(d\mu; x)$  in the form  $P_n(d\mu; x) = \sum_{q=0}^n k_q x^q$ , using the identity  $t^q - x^q = (t - x) \sum_{p=0}^{q-1} t^p x^{q-1-p}$ ,  $q = 1, 2, 3, \dots$  to cancel the denominator in Eq. (17) and noting that  $C_0(d\mu) > 0$ .  $\square$

**Definition 7** *The Stieltjes Transformation of the measure  $d\mu(x) = \bar{\mu}(x)dx$  is defined by[28]*

$$S_{\bar{\mu}}(z) = \int_a^b \frac{d\mu(x)}{z - x}, \quad (18)$$

where  $z \in \mathbb{C} - [a, b]$ .

**Theorem 5** *If a measure  $d\rho(x) = \rho(x)dx$  has Stieltjes transformation given by*

$$S_{\bar{\rho}}(z) = z - C_1(d\mu) - \frac{1}{S_{\bar{\mu}}(z)}, \quad (19)$$

*with  $C_0(d\mu) = 1$ , then the secondary polynomials  $\{Q_n(d\mu; x)\}_{n=1}^{\infty}$  form an orthogonal family for the induced inner product of  $d\rho(x)$ .*

*Proof* See [29], or [30] for a direct proof.

---

<sup>1</sup> also known as *polynomial of the second kind*.

## 2.2 Derivation of the sequence of secondary normalised measures

**Definition 8** For two measures  $d\rho(x)$  and  $d\mu(x)$  satisfying Eq. (19), we call  $d\rho(x)$  the secondary measure associated with  $d\mu(x)$ .

**Definition 9** We call the sequence of measures  $d\mu_0, d\mu_1, d\mu_2, \dots$  generated from a measure  $d\mu_0$  by

$$S_{\bar{\rho}_{n+1}}(z) = z - C_1(d\mu_n) - \frac{1}{S_{\bar{\mu}_n}(z)} \quad n = 0, 1, 2, \dots, \quad (20)$$

$$d\mu_n(x) = \bar{\mu}_n(x)dx \quad n = 0, 1, 2, \dots, \quad (21)$$

$$\bar{\mu}_n(x) = \frac{\bar{\rho}_n(x)}{C_0(d\rho_n)} \quad n = 1, 2, 3, \dots, \quad (22)$$

the sequence of normalised secondary measures, where  $C_0(d\mu_0) = 1$ .

**Corollary 2** All measures in a sequence of normalised secondary measures have their zeroth moment equal to unity.

*Proof* By taking zeroth moment of both sides of Eq. (22) we find

$$C_0(d\mu_n) = \frac{C_0(d\rho_n)}{C_0(d\rho_n)} = 1 \quad n = 1, 2, 3, \dots \quad (23)$$

We also have that  $C_0(d\mu_0) = 1$  by definition (9).  $\square$

**Lemma 2**

$$C_n(d\rho_{m+1}) = C_{n+2}(d\mu_m) - C_1(d\mu_m)C_{n+1}(d\mu_m) - \sum_{s=0}^{n-1} C_s(d\rho_{m+1})C_{n-s}(d\mu_m) \quad (24)$$

$n, m = 0, 1, 2, \dots$

*Proof* For simplifty we will prove Eq. (24) for  $m = 0$  as the generalisation is trivial. By Taylor expanding  $S_{\bar{\mu}_0}(z)$  and  $S_{\bar{\rho}_1}(z)$  in  $x = 1/z$  we find

$$S_{\bar{\mu}_0}(z) = \sum_{n=0}^{\infty} \frac{C_n(d\mu_0)}{z^{n+1}} \quad \text{as } z \rightarrow \infty, \quad (25)$$

$$S_{\bar{\rho}_1}(z) = \sum_{n=0}^{\infty} \frac{C_n(d\rho_1)}{z^{n+1}} \quad \text{as } z \rightarrow \infty. \quad (26)$$

From Eq. (19) we have

$$S_{\bar{\rho}_1}(z)S_{\bar{\mu}_0}(z) = (z - C_1(d\mu_0))S_{\bar{\rho}_1}(z) - 1. \quad (27)$$

Hence substituting Eq. (25) and (26) into Eq. (27) we find

$$\sum_{n,m=0}^{\infty} C_n(d\mu_0)C_m(d\rho_1)x^{n+m+2} = \left(\frac{1}{x} - C_1(d\mu_0)\right) \sum_{s=0}^{\infty} C_s(d\mu_0)x^{s+1} - 1. \quad (28)$$

By comparing terms of the same power in  $x$  and taking into account  $C_0(d\mu_0) = 1$  we deduce

$$\sum_{n=0}^m C_n(d\mu_0)C_{m-n}(d\rho_1) = C_{m+2}(d\mu_0) - C_1(d\mu_0)C_{m+1}(d\mu_0) \quad m = 0, 1, 2, \dots \quad (29)$$

By a change of variable in Eq. (29) we finally arrive at Eq. (24).  $\square$

**Lemma 3** *A sequence of normalised secondary measures  $d\mu_0, d\mu_1, d\mu_2, \dots, d\mu_n$ , can be written as a continued fraction of the form*

$$S_0(z) = \frac{1}{z - C_{1,0} - \frac{d_0}{z - C_{1,1} - \frac{d_1}{z - C_{1,2} - \frac{d_2}{\ddots \frac{d_{n-1}}{z - C_{1,n-1} - \frac{d_n S_{n+1}(z)}{z - C_{1,n} - d_n S_{n+1}(z)}}}}}} \quad (30)$$

where we have introduced the shorthand notation  $S_n(z) := S_{\bar{\mu}_n}(z)$ ,  $C_{n,s} := C_n(d\mu_s)$ ,  $n, s = 0, 1, 2, \dots$ ;  $d_n := C_{2,n} - C_{1,n}^2$ ,  $n = 1, 2, 3, \dots$ , and  $d_0 := 1$ .

*Proof* By evaluating Eq. (24) for  $n = 0$ , and taking into account the above definition of  $d_n$  we see that  $d_n = C(d\rho_n)$ ,  $n = 1, 2, 3, \dots$ . Using our new notation, Eq. (20) for the sequence of measures reads

$$S_{n+1}(z) = \frac{1}{d_n} \left[ z - C_{1,n} - \frac{1}{S_n(z)} \right], \quad n = 0, 1, 2, \dots \quad (31)$$

Solving this for  $S_n(z)$  followed by repeated substitution gives us Eq. (30).  $\square$

**Theorem 6** *The following relations hold for the continued fraction Eq. (30)*

$$S_0(z) = \frac{u_n(-d_n S_{n+1}(z)) + u_{n+1}}{v_n(-d_n S_{n+1}(z)) + v_{n+1}}, \quad n = 0, 1, 2, \dots, \quad (32)$$

with relations

$$u_{n+1} = (z - C_{1,n})u_n - d_{n-1}u_{n-1}, \quad v_{n+1} = (z - C_{1,n})v_n - d_{n-1}v_{n-1}, \quad (33)$$

and starting values

$$u_0 = 0, \quad u_1 = 1, \quad v_0 = 1, \quad v_1 = z - C_{0,1}. \quad (34)$$

*Proof* These are elementary results from the theory of continued fractions (e.g. see section 4, connection with continued fractions [31]).

**Lemma 4**

$$\Delta_{n+1} := u_{n+1}v_n - v_{n+1}u_n = d_0 d_1 d_2 \dots d_{n-1}, \quad n = 1, 2, 3, \dots, \quad (35)$$

$$\Delta_1 = 1. \quad (36)$$



*Proof* Using Eq. (33) to substitute for  $u_{n+1}$  and  $v_{n+1}$  into Eq. (35), we find the relation  $\Delta_{n+1} = d_{n-1}\Delta_n$ . Using Eq. (34) to verify Eq. (35) for the starting values, Eq. (35) follows by induction.  $\square$

**Definition 10** A Padé Approximant for a function  $g$  of type  $q/p$  in the neighbourhood of 0 is a rational fraction

$$F(z) = \frac{Q(z)}{P(z)}, \quad (37)$$

with degree of  $Q \leq q$ , degree of  $P \leq p$  and  $g(z) - \frac{Q(z)}{P(z)}$  of order  $\mathcal{O}(z^{p+q+1})$  in the neighbourhood of 0.

For more details, see [31].

**Theorem 7**  $F_n(z) = \frac{u_{n+1}(z)}{v_{n+1}(z)}$  is a Padé Approximant for  $S_0(z)$  of type  $n/(n+1)$ ,  $n = 0, 1, 2, \dots$ .

*Proof* Using theorem (6), we can write  $S_0(z) - \frac{u_{n+1}(z)}{v_{n+1}(z)}$  as

$$S_0(z) - \frac{u_{n+1}(z)}{v_{n+1}(z)} = \frac{\Delta_{n+1}d_n S_{n+1}(z)}{v_{n+1}(z)(v_{n+1}(z) - d_n v_n(z)S_{n+1}(z))}, \quad n = 0, 1, 2, \dots \quad (38)$$

Through lemma (4) we see that  $\Delta_{n+1}$  is independent of  $z$ . By Taylor expanding  $S_{n+1}(z)$  defined in definition (7) about  $x = 1/z$ , and remembering that  $C_0(d\mu_n) = 1$   $n = 1, 2, 3, \dots$ , we find using Eq. (38) that

$$S_{n+1}(z) = \frac{1}{z} + \mathcal{O}\left(\frac{1}{z^2}\right) \quad \text{as } z \rightarrow \infty \quad n = 0, 1, 2, \dots \quad (39)$$

By induction, we see that  $v_{n+1}$  and  $u_{n+1}$ ,  $n = 0, 1, 2, \dots$  given by Eq. (33) and (34), are degree  $n+1$  and  $n$  polynomials in  $z$  respectively, both with leading coefficients equal to unity. Hence we conclude that

$$S_0(z) - \frac{u_{n+1}(z)}{v_{n+1}(z)} = \frac{\Delta_{n+1}d_n}{z^{2n+3}} = \frac{d_0d_1 \dots d_n}{z^{2n+3}} \quad \text{as } z \rightarrow \infty \quad n = 0, 1, 2, \dots \quad (40)$$

Thus by definition (10) we conclude the proof.  $\square$

**Lemma 5**  $u_n(z) = \lambda_n Q_n(d\mu_0; z)$  and  $v_n(z) = \lambda_n P_n(d\mu_0; z)$   $n = 0, 1, 2, \dots$ , with  $\lambda_n = 1/a_n$  where  $a_n$  is defined in definition (4).

*Proof* From section 5.3.: moment problems and orthogonal polynomials (p213-220) of [31], and theorem (7) it follows that

$$\frac{u_{n+1}(z)}{v_{n+1}(z)} = \frac{Q_{n+1}(d\mu_0; z)}{P_{n+1}(d\mu_0; z)} \quad n = 0, 1, 2, \dots \quad (41)$$

By observing the starting values, we also have that

$$\frac{u_0(z)}{v_0(z)} = \frac{Q_0(d\mu_0; z)}{P_0(d\mu_0; z)}. \quad (42)$$

Hence

$$u_n(z) = \lambda_n Q_n(d\mu_0; z) \quad \text{and} \quad v_n(z) = \lambda_n P_n(d\mu_0; z) \quad n = 0, 1, 2, \dots \quad (43)$$

Given that  $u_n$  and  $v_n$  have leading coefficients equal to 1, we must have  $\lambda_n = 1/a_n$   $n=0, 1, 2, \dots$ .  $\square$

**Theorem 8**  $d_n = a_n^2/a_{n+1}^2 = \beta_{n+1}(d\mu_0) \quad n = 0, 1, 2, \dots$

*Proof* Proceeding in the same way as in page (18) of [27], we have

$$S_0(z) - \frac{Q_n(d\mu_0; z)}{P_n(d\mu_0; z)} = \frac{\gamma_n}{z^{2n+1}} \quad \text{as } z \rightarrow \infty \quad n = 0, 1, 2, \dots \quad (44)$$

where

$$\gamma_n = \frac{1}{a_n} \int_a^b x^n P_n(d\mu_0; x) d\mu_0(x) = \frac{\gamma_0 a_0^2}{a_n^2} \frac{\langle P_n(d\mu_0), P_n(d\mu_0) \rangle_{\bar{\mu}}}{\langle P_0(d\mu_0), P_0(d\mu_0) \rangle_{\bar{\mu}}} \quad n = 0, 1, 2, \dots \quad (45)$$

Noting that  $P_0(d\mu_0; x)/a_0 = \pi_0(d\mu_0; x) = 1$  and that  $C_0(d\mu_0) = 1$ , Eq. (45) tells us  $\gamma_0 = 1$ . Comparing Eq. (44) with Eq. (40) and (41), we deduce that

$$d_0 d_1 \dots d_{n-1} = \frac{a_0^2}{a_n^2} \frac{\langle P_n(d\mu_0), P_n(d\mu_0) \rangle_{\bar{\mu}}}{\langle P_0(d\mu_0), P_0(d\mu_0) \rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots \quad (46)$$

By induction it follows

$$d_n = \frac{a_n^2}{a_{n+1}^2} \frac{\langle P_{n+1}(d\mu_0), P_{n+1}(d\mu_0) \rangle_{\bar{\mu}}}{\langle P_n(d\mu_0), P_n(d\mu_0) \rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots \quad (47)$$

Due to definition (3), we see that  $\langle P_n(d\mu_0), P_n(d\mu_0) \rangle_{\bar{\mu}} = 1 \quad n = 0, 1, 2, \dots$ , hence

$$d_n = \frac{a_n^2}{a_{n+1}^2} \quad n = 1, 2, 3, \dots \quad (48)$$

From definition (4), we see that Eq. (47) can be written in the form

$$d_n = \frac{\langle \pi_{n+1}(d\mu_0), \pi_{n+1}(d\mu_0) \rangle_{\bar{\mu}}}{\langle \pi_n(d\mu_0), \pi_n(d\mu_0) \rangle_{\bar{\mu}}} \quad n = 1, 2, 3, \dots \quad (49)$$

Hence, from definition (8) we conclude,

$$d_n = \beta_{n+1}(d\mu_0) \quad n = 1, 2, 3, \dots \quad (50)$$

For  $n = 1$ , Eq. (46) gives us

$$d_0 = \frac{\langle \pi_1(d\mu_0), \pi_1(d\mu_0) \rangle_{\bar{\mu}}}{\langle \pi_0(d\mu_0), \pi_0(d\mu_0) \rangle_{\bar{\mu}}} = \frac{a_0^2}{a_1^2} = \beta_1(d\mu_0). \quad (51)$$

□

**Theorem 9** *Measures  $d\mu(x) = \bar{\mu}(x)dx$  can be calculated from their Stieltjes transform by*

$$\bar{\mu}(x) = \frac{1}{2\pi i} \lim_{\epsilon \rightarrow 0^+} [S_{\bar{\mu}}(x - i\epsilon) - S_{\bar{\mu}}(x + i\epsilon)]. \quad (52)$$

*Proof* This result is known as the *Stieltjes-Perron inversion formula*. See [32].

**Definition 11** *We call  $\varphi(d\mu; x)$  the reducer of measure  $d\mu(x)$ . It is given by*

$$\varphi(d\mu; x) = \lim_{\epsilon \rightarrow 0^+} [S_{\bar{\mu}}(x - i\epsilon) + S_{\bar{\mu}}(x + i\epsilon)]. \quad (53)$$

The reducer allows us to write an explicit expression for the secondary measure associated with  $\bar{\mu}(x)$  as follows.

**Theorem 10** *For a measure  $d\mu(x)$  with secondary measure  $d\rho(x)$ , we have*

$$\bar{\rho}(x) = \frac{\bar{\mu}(x)}{\frac{\varphi^2(d\mu; x)}{4} + \pi^2 \bar{\mu}^2(x)} \quad (54)$$

*Proof* See [30].

**Definition 12** *We define the functions  $Z_n(x) \in \mathbb{C} \quad n = 0, 1, 2, \dots$  as*

$$Z_n(x) = \frac{\varphi_n(x)}{2} + i\pi \bar{\mu}_n(x) \quad n = 0, 1, 2, \dots, \quad (55)$$

where  $\varphi_n(x) := \varphi(d\mu_n; x)$ .

**Lemma 6** *The following recursion relation hold for  $Z_{n+1}(x)$*

$$Z_{n+1}(x) = \frac{1}{d_n} [x - C_{1,n} - \frac{1}{Z_n(x)}], \quad n = 0, 1, 2, \dots \quad (56)$$

*Proof* We start by finding a relation between the Stieltjes transformation of a measure  $d\mu(x)$ , and the reducer of its associated secondary measure  $d\rho(x)$ : By definition, we have

$$\varphi(d\rho; x) = \lim_{\epsilon \rightarrow 0^+} [S_{\bar{\rho}}(x - i\epsilon) + S_{\bar{\rho}}(x + i\epsilon)]. \quad (57)$$

Using Eq. (19), we find

$$\varphi(d\rho; x) = 2[x - C_1(d\mu)] - \lim_{\epsilon \rightarrow 0^+} \frac{S_{\bar{\mu}}(x - i\epsilon) + S_{\bar{\mu}}(x + i\epsilon)}{S_{\bar{\mu}}(x - i\epsilon)S_{\bar{\mu}}(x + i\epsilon)}. \quad (58)$$

Now using theorem (9) and definition (11), we find that

$$\lim_{\epsilon \rightarrow 0^+} \frac{S_{\bar{\mu}}(x - i\epsilon) + S_{\bar{\mu}}(x + i\epsilon)}{S_{\bar{\mu}}(x - i\epsilon)S_{\bar{\mu}}(x + i\epsilon)} = \frac{\varphi(d\mu; x)}{\frac{\varphi^2(d\mu; x)}{4} + \pi^2 \bar{\mu}^2(x)}. \quad (59)$$

Hence from Eq. (58) we get

$$\varphi(d\rho; x) = 2[x - C_1(d\mu)] - \frac{\varphi(d\mu; x)}{\frac{\varphi^2(d\mu; x)}{4} + \pi^2 \bar{\mu}^2(x)}. \quad (60)$$

Using the definition of a sequence of normalised secondary measures, definition (9) and the definition of  $d_n$  in Lemma (3), from Eq. (60) we find

$$\varphi_{n+1}(x) = \frac{1}{d_n} \left[ 2[x - C_{1,n}] - \frac{\varphi_n(x)}{\frac{\varphi_n^2(x)}{4} + \pi^2 \bar{\mu}_n^2(x)} \right], \quad n = 0, 1, 2, \dots \quad (61)$$

Similarly, we can also write theorem (10) for our sequence of normalised secondary measures using definition (9) and  $d_n$ . We find

$$\bar{\mu}_{n+1}(x) = \frac{1}{d_n} \left[ \frac{\bar{\mu}_n(x)}{\frac{\varphi_n^2(x)}{4} + \pi^2 \bar{\mu}_n^2(x)} \right], \quad n = 0, 1, 2, \dots \quad (62)$$

If we write Eq. (55) for  $Z_{n+1}(x)$  and then substitute Eq. (61) and Eq. (62) into the RHS we arrive at Eq. (56).  $\square$

**Theorem 11** *The following relations hold between  $Z_0(x)$  and  $Z_{n+1}(x)$*

$$Z_0(z) = \frac{u_n(-d_n Z_{n+1}(z)) + u_{n+1}}{v_n(-d_n Z_{n+1}(z)) + v_{n+1}}, \quad n = 0, 1, 2, \dots, \quad (63)$$

where  $u_n(z) = \lambda_n Q_n(d\mu_0; z)$  and  $v_n(z) = \lambda_n P_n(d\mu_0; z)$   $n = 0, 1, 2, \dots$ , with  $\lambda_n = 1/a_n$ ,  $a_n$  defined in definition (4).

*Proof* By comparing Eq. (56) with eq. (31), we note that  $Z_n(x)$  satisfies the same recursion relation as  $S_n(x)$ . Hence theorem (32) readily applies to Eq. (56) if we exchange  $S_{n+1}(x)$  with  $Z_{n+1}(x)$  and  $S_0(x)$  with  $Z_0(x)$ . The relations between  $u_n$ ,  $v_n$  and  $Q_n$ ,  $P_n$  are proven in lemma (5).  $\square$

We are now ready to state our first main theorem:

**Theorem 12** *A sequence of normalised secondary measures starting from  $d\mu_0$ :  $d\mu_0$ ,  $d\mu_1$ ,  $d\mu_2, \dots$ ,  $d\mu_m, \dots$  can be generated from the first measure in the sequence  $d\mu_0$  by the formula*

$$\bar{\mu}_n(x) = \frac{1}{t_{n-1}^2(d\mu_0)} \frac{\bar{\mu}_0(x)}{\left(P_{n-1}(d\mu_0; x) \frac{\varphi(d\mu_0; x)}{2} - Q_{n-1}(d\mu_0; x)\right)^2 + \pi^2 \bar{\mu}_0^2(x) P_{n-1}^2(d\mu_0; x)} \quad (64)$$

$n = 1, 2, 3, \dots$ ,

where the  $t_n$  coefficients are defined in definition (4).

*Proof* After solving Eq. (63) for  $Z_n(x)$ , we find

$$Z_n(x) = \frac{a_{n-1}}{a_n d_{n-1}} \frac{Z_0(x) P_n(d\mu_0; x) - Q_n(d\mu_0; x)}{Z_0(x) P_{n-1}(d\mu_0; x) - Q_{n-1}(d\mu_0; x)} \quad n = 1, 2, 3, \dots \quad (65)$$

From theorem (8) we see that

$$a_{n-1}/a_n = \kappa_n \sqrt{d_{n-1}} \quad n = 1, 2, 3, \dots, \quad (66)$$

where  $\kappa_n$  is the sign of  $a_{n-1}/a_n$ . After using this relation to simplify the  $a_{n-1}/a_n d_{n-1}$  coefficient in Eq. (65) and substituting for  $Z_0(x)$  using definition (12), we take real and imaginary parts to achieve

$$\bar{\mu}_n(x) = \frac{\kappa_n}{\sqrt{d_{n-1}}} \frac{\bar{\mu}_0(x) [P_{n-1}(d\mu_0; x) Q_n(d\mu_0; x) - P_n(d\mu_0; x) Q_{n-1}(d\mu_0; x)]}{\left(P_{n-1}(d\mu_0; x) \frac{\varphi(d\mu_0; x)}{2} - Q_{n-1}(d\mu_0; x)\right)^2 + \pi^2 \bar{\mu}_0^2(x) P_{n-1}^2(d\mu_0; x)} \quad (67)$$

$n = 1, 2, 3, \dots$ . Using the identities from lemmas (4) and (5), we note that

$$P_n(d\mu_0; x) Q_{n+1}(d\mu_0; x) - P_{n+1}(d\mu_0; x) Q_n(d\mu_0; x) = d_0 d_1 \dots d_{n-1} / \lambda_n \lambda_{n+1} \quad (68)$$

$n = 1, 2, 3, \dots$ . Using theorem (8) and lemma (5) to write the RHS in terms of the  $a_n$ 's, we find

$$d_0 d_1 \dots d_{n-1} / \lambda_n \lambda_{n+1} = a_0^2 a_{n+1} / a_n = a_0^2 / \kappa_{n+1} \sqrt{d_n} \quad n = 0, 1, 2, \dots, \quad (69)$$

where in the last line we have used Eq. (66). We now note that by definition (4),  $P_0(d\mu_0; x) = a_0$ . We also have by definition (3), that  $\langle P_0(d\mu_0; x), P_0(d\mu_0; x) \rangle_{\bar{\mu}_0} = 1$ . Hence

$$1 = \langle P_0(d\mu_0; x), P_0(d\mu_0; x) \rangle_{\bar{\mu}_0} = a_0^2 C_0(d\mu_0) = a_0^2. \quad (70)$$

Hence from Eq. (68), (69), (70), we find that we can write Eq. (67) as

$$\bar{\mu}_n(x) = \frac{1}{d_{n-1}} \frac{\bar{\mu}_0(x)}{\left( P_{n-1}(d\mu_0; x) \frac{\varphi(d\mu_0; x)}{2} - Q_{n-1}(d\mu_0; x) \right)^2 + \pi^2 \bar{\mu}_0^2(x) P_{n-1}^2(d\mu_0; x)} \quad (71)$$

$n = 1, 2, 3, \dots$ . Finally, with the relations from theorems (8) and (4) we find  $d_{n-1} = t_{n-1}^2(d\mu_0)$   $n = 1, 2, 3, \dots$ .  $\square$

### 2.3 Derivation of the Jacobi matrix theorem

**Lemma 7** *The  $\alpha_n(d\mu)$  and  $\beta_n(d\mu)$  coefficients defined in theorem (2) are invariant under a change of scale of the measure  $d\mu(x)$ , while the change in  $\beta_0(d\mu)$  scales linearly:*

$$\alpha_n(Cd\mu) = \alpha_n(d\mu) \quad n = 0, 1, 2, \dots \quad (72)$$

$$\beta_n(Cd\mu) = \beta_n(d\mu) \quad n = 1, 2, 3, \dots \quad (73)$$

$$\beta_0(Cd\mu) = C\beta_0(d\mu) \quad (74)$$

where  $C > 0$ .

*Proof* First we will show that  $\pi_n(Cd\mu; x) = \pi_n(d\mu; x)$   $n = 0, 1, 2, \dots$ . From definition (4), we have that

$$1 = \langle P_n(d\mu), P_n(d\mu) \rangle_{\bar{\mu}} \quad n = 0, 1, 2, \dots \quad (75)$$

By multiplying and dividing by  $C$  we find

$$1 = \left\langle \frac{P_n(d\mu)}{\sqrt{C}}, \frac{P_n(d\mu)}{\sqrt{C}} \right\rangle_{C\bar{\mu}} \quad n = 0, 1, 2, \dots \quad (76)$$

From definition (4), we conclude

$$P_n(Cd\mu; x) = \frac{P_n(d\mu; x)}{\sqrt{C}} \quad n = 0, 1, 2, \dots \quad (77)$$

By observing definition (4) and Eq. (77), we conclude

$$a_n(Cd\mu) = a_n(d\mu)/\sqrt{C} \quad n = 0, 1, 2, \dots \quad (78)$$

Hence, from Eq. (77), (78) and definition (4) it follows

$$\pi_n(Cd\mu; x) = P_n(Cd\mu; x)/a_n(Cd\mu) = P_n(d\mu; x)/a_n(d\mu) = \pi_n(d\mu; x) \quad (79)$$

$n = 0, 1, 2, \dots$ . Now we can see how the  $\alpha_n$  and  $\beta_n$  coefficients change:  
Using definition (2) and Eq. (79) we have

$$\alpha_n(Cd\mu) = \frac{\langle x\pi_n(Cd\mu), \pi_n(Cd\mu) \rangle_{\bar{C}\bar{\mu}}}{\langle \pi_n(Cd\mu), \pi_n(Cd\mu) \rangle_{\bar{C}\bar{\mu}}} \quad (80)$$

$$= \frac{\langle x\pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}}{\langle \pi_n(d\mu), \pi_n(d\mu) \rangle_{\bar{\mu}}} \quad (81)$$

$$= \alpha_n(d\mu), \quad n = 0, 1, 2, \dots \quad (82)$$

Similarly, we find

$$\beta_n(Cd\mu) = \beta_n(d\mu), \quad n = 1, 2, 3, \dots \quad (83)$$

In the case of  $\beta_0$  we have

$$\beta_0(Cd\mu) = \langle \pi_0(Cd\mu), \pi_0(Cd\mu) \rangle_{\bar{C}\bar{\mu}} = C\beta_0(d\mu). \quad (84)$$

□

**Theorem 13** *If  $d\rho(x)$  is the secondary measure associated with  $d\mu(x)$ , then*

$$\alpha_{n+1}(d\mu) = \alpha_n(d\rho) \quad n = 0, 1, 2, \dots \quad (85)$$

$$\beta_{n+1}(d\mu) = \beta_n(d\rho) \quad n = 1, 2, 3, \dots \quad (86)$$

*Proof* See [27], theorem 1.36 (page 16).

**Lemma 8** *A sequence of normalised secondary measures  $d\mu_0(x)$ ,  $d\mu_1(x)$ ,  $d\mu_2(x)$ ,  $\dots$ , satisfy*

$$\alpha_{m+n}(d\mu_0) = \alpha_n(d\mu_m) \quad n, m = 0, 1, 2, \dots, \quad (87)$$

$$\beta_{m+n}(d\mu_0) = \beta_n(d\mu_m) \quad n = 1, 2, 3, \dots, m = 0, 1, 2, \dots \quad (88)$$

*Proof* Using lemma (7) and definition (9) we find

$$\alpha_n(d\rho_m) = \alpha_n(d\rho_m/C_0(d\rho_m)) = \alpha_n(d\mu_m) \quad n = 0, 1, 2, \dots, m = 1, 2, 3, \dots, \quad (89)$$

$$\beta_n(d\rho_m) = \beta_n(d\rho_m/C_0(d\rho_m)) = \beta_n(d\mu_m) \quad n = 1, 2, 3, \dots, m = 1, 2, 3, \dots \quad (90)$$

Hence taking into account theorem (13) we find

$$\alpha_{n+1}(d\mu_p) = \alpha_n(d\mu_{p+1}) \quad n, p = 0, 1, 2, \dots, \quad (91)$$

$$\beta_{n+1}(d\mu_p) = \beta_n(d\mu_{p+1}) \quad n = 1, 2, 3, \dots, p = 0, 1, 2, \dots \quad (92)$$

We will now proceed to prove Eq. (87) by construction: by evaluating Eq. (91), for  $(n, p)$  at  $(s-1, m)$ ,  $(s-2, m+1)$ ,  $(s-3, m+2)$ ,  $\dots$ ,  $(0, m+s-1)$  for any  $m \geq 0$ ,  $s \geq 1$  we have the following sequence of equations

$$\alpha_s(d\mu_m) = \alpha_{s-1}(d\mu_{m+1}) \quad (93)$$

$$\alpha_{s-1}(d\mu_{m+1}) = \alpha_{s-2}(d\mu_{m+2}) \quad (94)$$

$$\alpha_{s-2}(d\mu_{m+2}) = \alpha_{s-3}(d\mu_{m+3}) \quad (95)$$

$\vdots$

$$\alpha_1(d\mu_{m+s-1}) = \alpha_0(d\mu_{m+s}). \quad (96)$$

Thus by repeated substitution we arrive at

$$\alpha_s(d\mu_m) = \alpha_0(d\mu_{m+s}), \quad m = 0, 1, 2, \dots, s = 1, 2, 3, \dots \quad (97)$$

We note that this equation is also valid for  $s = 0$ . If we make the change of variable  $s = p + n$ ,  $m = 0$  in Eq. (97) followed by relabeling indices, we find

$$\alpha_{m+s}(d\mu_0) = \alpha_0(d\mu_{m+s}) \quad m, s = 0, 1, 2, \dots \quad (98)$$

Hence from Eq. (97) and (98), we arrive at (87). Similarly, we prove Eq. (88).  $\square$

**Definition 13** We call the sequence of measures  $d\nu_0(x)$ ,  $d\nu_1(x)$ ,  $d\nu_2(x)$ ,  $d\nu_3(x)$ , ... beta normalised measures, where  $d\nu_0(x)$  defines the sequence

$$\bar{\nu}_n(x) = \frac{\bar{\nu}_0(x)}{\left(P_{n-1}(d\nu_0; x) \frac{\varphi(d\nu_0; x)}{2} - Q_{n-1}(d\nu_0; x)\right)^2 + \pi^2 \bar{\nu}_0^2(x) P_{n-1}^2(d\nu_0; x)} \quad (99)$$

$n = 1, 2, 3, \dots$ , and  $d\nu_n(x) = \bar{\nu}_n(x) dx \quad n = 0, 1, 2, \dots$

**Lemma 9** For every sequence of beta normalised measures  $\{d\nu_n\}_{n=0}^{n=\infty}$ , there always exists a sequence of normalised secondary measures  $\{d\mu_n\}_{n=0}^{n=\infty}$  such that

$$\bar{\nu}_n(x) = \beta_n(d\nu_0) \bar{\mu}_n(x) \quad n = 0, 1, 2, \dots \quad (100)$$

*Proof* For  $n = 0$  in Eq. (100) and taking into account corollary (1), we have

$$\bar{\nu}_0(x) = C_0(d\nu_0) \bar{\mu}_0(x). \quad (101)$$

The only additional constraint on  $d\mu_0$  as compared with any measure  $d\mu$ , is that  $C_0(d\mu_0) = 1$ . By calculating the zeroth moment of both sides, we see that relation Eq. (101) satisfies this additional constraint. Now we will proceed by finding an expression for the sequence of normalised measures generated from  $d\mu_0$  in terms of  $d\nu_0$ . For this we need to find how the quantities  $P_n(d\mu_0; x)$ ,  $Q_n(d\mu_0; x)$ ,  $\beta_{n+1}(d\mu_0)$ ,  $n = 0, 1, 2, \dots$  and  $\varphi(d\mu_0; x)$  can be written in terms of  $P_n(d\nu_0; x)$ ,  $Q_n(d\nu_0; x)$ ,  $\beta_{n+1}(d\nu_0)$ ,  $n = 0, 1, 2, \dots$  and  $\varphi(d\nu_0; x)$  respectively. Using relation Eq. (101) and definition (3), we find

$$P_n(d\mu_0; x) = \sqrt{C_0(d\nu_0)} P_n(d\nu_0; x) \quad n = 0, 1, 2, \dots \quad (102)$$

Using this relation, and definitions (6) and (11), we find

$$Q_n(d\mu_0; x) = \frac{Q_n(d\nu_0; x)}{\sqrt{C_0(d\nu_0)}} \quad n = 0, 1, 2, \dots, \quad (103)$$

$$\varphi(d\mu_0; x) = \frac{\varphi(d\nu_0; x)}{C_0(d\nu_0)}. \quad (104)$$

Lemma (7) tells us

$$\beta_n(d\mu_0) = \beta_n(d\nu_0) \quad n = 1, 2, 3, \dots \quad (105)$$

Hence using relation Eq. (16), we find

$$t_{n-1}^2(d\mu_0) = t_{n-1}^2(d\nu_0) = \beta_n(d\nu_0) \quad n = 1, 2, 3, \dots \quad (106)$$

Now substituting Eq. (102), (103), (104), and (106) into Eq. (64),

$$\bar{\mu}_n(x) = \frac{1}{\beta_n(d\nu_0)} \frac{\bar{\nu}_0(x)}{\left(P_{n-1}(d\nu_0; x) \frac{\varphi(d\nu_0; x)}{2} - Q_{n-1}(d\nu_0; x)\right)^2 + \pi^2 \bar{\nu}_0^2(x) P_{n-1}^2(d\nu_0; x)} \quad (107)$$

$n = 1, 2, 3, \dots$ . Hence by observing definition (13), we find Eq. (100) for  $n = 1, 2, 3, \dots$ .  $\square$

**Theorem 14** *A sequence of beta normalised measures  $d\nu_0(x)$ ,  $d\nu_1(x)$ ,  $d\nu_2(x)$ ,  $\dots$ , satisfy*

$$\alpha_{m+n}(d\nu_0) = \alpha_n(d\nu_m) \quad n, m = 0, 1, 2, \dots, \quad (108)$$

$$\beta_{m+n}(d\nu_0) = \beta_n(d\nu_m) \quad n, m = 0, 1, 2, \dots. \quad (109)$$

*Proof* From lemma (9) we see that  $d\mu_n$  and  $d\nu_n$  are related by a constant, hence using lemmas (7) and (8) we find

$$\alpha_{m+n}(d\nu_0) = \alpha_n(d\nu_m) \quad n, m = 0, 1, 2, \dots, \quad (110)$$

$$\beta_{m+n}(d\nu_0) = \beta_n(d\nu_m) \quad n = 1, 2, 3, \dots, m = 0, 1, 2, \dots. \quad (111)$$

For  $\beta_0(d\nu_m)$  we find

$$\beta_0(d\nu_m) = \beta_0(\beta_m(d\nu_0)d\mu_m) = \beta_m(d\nu_0)C_0(d\mu_m) \quad m = 0, 1, 2, \dots, \quad (112)$$

where we have used Eq. (100) followed by Eq. (74) and then corollary (1). But  $C_0(d\mu_m) = 1$   $m = 0, 1, 2, \dots$ , by definition.  $\square$

*Remark 1* As we will see in section 4, for a wide range of  $d\nu_0$ ;  $\alpha_{m+n}(d\nu_0)$ ,  $\beta_{m+n}(d\nu_0)$  and  $d\nu_m$  can be determined analytically. Hence Eq. (108) and Eq. (109) can also be used to find analytical solutions to a wide range of integrals.

**Definition 14** *We will call the infinite tridiagonal matrix of a measure  $d\mu(x)$*

$$\mathcal{J}(d\mu) = \begin{bmatrix} \alpha_0(d\mu) & \sqrt{\beta_1(d\mu)} & & & 0 \\ \sqrt{\beta_1(d\mu)} & \alpha_1(d\mu) & \sqrt{\beta_2(d\mu)} & & \\ & \sqrt{\beta_2(d\mu)} & \alpha_2(d\mu) & \sqrt{\beta_3(d\mu)} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{bmatrix}, \quad (113)$$

the Jacobi matrix. See [27] for more details.

**Definition 15** *We will call the matrix*

$$\mathcal{J}_n(d\mu) = \begin{bmatrix} \alpha_n(d\mu) & \sqrt{\beta_{n+1}(d\mu)} & & & 0 \\ \sqrt{\beta_{n+1}(d\mu)} & \alpha_{n+1}(d\mu) & \sqrt{\beta_{n+2}(d\mu)} & & \\ & \sqrt{\beta_{n+2}(d\mu)} & \alpha_{n+2}(d\mu) & \sqrt{\beta_{n+3}(d\mu)} & \\ & & \ddots & \ddots & \ddots \\ 0 & & & & \end{bmatrix} \quad (114)$$

$n = 1, 2, 3, \dots$ , the  $n$ th associated Jacobi matrix of the Jacobi matrix  $\mathcal{J}(d\mu)$ .



We are now ready to state our second main theorem:

**Theorem 15** *For Jacobi matrices for which its corresponding measure defines a sequence of normalised secondary measures, there exist an infinite sequence of associated Jacobi matrices corresponding to the sequence of normalised secondary measures. These matrices are formed by crossing-out the first row and column of the previous Jacobi matrix in the sequence:*

$$\mathcal{J}_n(d\mu_0) = \mathcal{J}(d\mu_n) \quad n = 1, 2, 3, \dots \quad (115)$$

*Proof* By equating the matrix elements in Eq. (115), we find Eq. (87) and (88). Hence lemma (8) implies Eq. (115).  $\square$

**Corollary 3** *Theorem (15) is also valid for any sequence of measures which are proportional to a sequence of normalised secondary measures such as the beta normalised measures.*

*Proof* Given that the Jacobi matrix does not contain the  $\beta_0$  coefficient, the result follows easily from lemma (7).  $\square$

### 3 Chain mappings of open quantum systems and Markovian embeddings

#### 3.1 Generalised mapping

An open quantum system can be represented by a system plus bath (also known as environment) model introduced by Caldeira and Leggett [33]. The Hamiltonian for this model is

$$H = H_S + H_E + H_{int}, \quad (116)$$

where  $H_S$  is the Hamiltonian which governs the system dynamics,  $H_E$  is the Hamiltonian of the environment and  $H_{int}$  describes the interaction between the two. In the case where the environment has a continuous set of degrees of freedom and the interaction between the system and environment is linear and does not depend on the state of the system, we can write the Hamiltonian as

$$H = H_S + H_E + H_{int} = H_S + \int_{x_{min}}^{x_{max}} dx g(x) a_x^\dagger a_x + \int_{x_{min}}^{x_{max}} dx A h(x) (a_x^\dagger + a_x). \quad (117)$$

where  $g(x), h(x) \in \mathbb{R}$  and have real domain  $[x_{min}, x_{max}]$ .  $A$  is an arbitrary hermitian operator acting on the system part of the Hilbert space. The set of operators  $\{a_x, a_x^\dagger\}$ ,  $x \in [x_{min}, x_{max}]$  are creation and annihilation operators and hence satisfy  $[a_x, a_y^\dagger] = \delta(x - y)$ . Physically  $g(x)$  represents the dispersion relation of the environment and  $h(x)$  determines the system-environment coupling strength. Together they determine the spectral density in the following way

**Definition 16** *We call the function  $J(x)$  the spectral density,*

$$J(\omega) = \pi h^2 [g^{-1}(\omega)] \frac{dg^{-1}(\omega)}{d\omega}, \quad (118)$$

where  $g^{-1}(g(x)) = g(g^{-1}(x)) = x$ ,  $\text{Dom}[J] \in [0, \omega_{max}]$ , and  $J(\omega) \geq 0$  its domain. For cases where  $\omega_{max} = \infty$ , we adapt the definition of the domain in an obvious way.

*Remark 2* As we will see later in the proof to theorem (16) (more specifically in Eq. 145), we use the  $J(x)$  function in the definition of a measure  $M(x)$  in such a way that  $M(x) = 0$  if  $J(x) = 0$ . Hence if we want to form a valid measure according to definition (1), we need  $J(x) > 0$  over its domain. For cases where this does not hold and  $J(x)$  is zero at a point(s) in the interval  $(0, \omega_{max})$ , we can define a set of spectral densities by redefining their domain such that they contain only non positive values at the boundaries of their domain. Also see remark (6).

The influence of the environment on the reduced system's dynamics is uniquely determined by  $J(x)$  when the initial state of the environment is gaussian [10]. Consequently, Eq. (118) tells us that a specific choice of  $g(x)$  does not determine uniquely the system's dynamics when the initial state on the environment is gaussian. This freedom of choice of  $g(x)$  will be vital in the proof of theorem (16), which is our third main theorem. We should also note that theorem (16) is also valid for any initial environment state if the  $g(x)$  and  $h(x)$  functions found in Eq. (142) and Eq. (144) respectively, are equal to the  $g(x)$  and  $h(x)$  in the initial Hamiltonian, i.e. Eq. (119).

**Theorem 16** *A system linearly coupled with a reservoir characterized by a spectral density  $J(x)$  is unitarily equivalent to semi-infinite chains with only nearest-neighbors interactions, where the system only couples to the first site in the chain. In other words, starting from an initial Hamiltonian,*

$$H = H_S + H_E + H_{int} = H_S + \int_{x_{min}}^{x_{max}} dx g(x) a_x^\dagger a_x + \int_{x_{min}}^{x_{max}} dx A h(x) (a_x^\dagger + a_x), \quad (119)$$

there exists a unitary operator  $\{U_n(x)\}_{n=0}^\infty$  such that the countably infinite set of new operators

$$b_n^\dagger = \int_{x_{min}}^{x_{max}} dx U_n(x) a_x^\dagger \quad n = 0, 1, 2, \dots, \quad (120)$$

satisfy the corresponding commutation relations

$$[b_n, b_m^\dagger] = \delta_{nm} \quad n, m = 0, 1, 2, \dots, \quad (121)$$

with transformed Hamiltonian

$$H \mapsto H_S + H_{E,q} + H_{int,q}, \quad (122)$$

$$H_{E,q} = \sum_{n=0}^{\infty} \left\{ E_{1n}(q) (e^{2iA_2} b_n^\dagger b_n^\dagger + e^{-2iA_2} b_n b_n) + E_{2n}(q) b_n^\dagger b_n \right. \quad (123)$$

$$\left. + E_{3n}(q) (e^{2iA_2} b_n^\dagger b_{n+1}^\dagger + e^{-2iA_2} b_n b_{n+1}) \right. \quad (124)$$

$$\left. + E_{4n}(q) (b_n^\dagger b_{n+1} + b_n b_{n+1}^\dagger) \right\}, \quad (125)$$

$$H_{int,q} = E_{5n}(q) A (e^{iA_2} b_0^\dagger + e^{-iA_2} b_0). \quad (126)$$

where  $E_{1n}(q)$ ,  $E_{2n}(q)$ ,  $E_{3n}(q)$ ,  $E_{4n}(q)$ ,  $E_{5n}(q)$ ,  $A_2 \in \mathbb{R}$  and  $q \in [0, 1]$  is a free parameter of the mapping which determines the particular version. For a pictorial representation of this theorem, see (a) and (b) of figure (1).

*Proof* The proof is by construction.

Let us start by defining the most general type of transformation of the creation and annihilation operators  $a_x^\dagger$  and  $a_x$  in terms of another set,  $c_x$  and  $c_x^\dagger$ , which preserves the commutation relations. We can do this via the so called *Bogoliubov transformation*[34]

$$a_x = e^{i\theta_1(x)} \cosh(r(x))c_x + e^{i\theta_2(x)} \sinh(r(x))c_x^\dagger, \quad (127)$$

$$a_x^\dagger = e^{-i\theta_1(x)} \cosh(r(x))c_x^\dagger + e^{-i\theta_2(x)} \sinh(r(x))c_x, \quad (128)$$

where  $\theta_1(x), \theta_2(x), r(x) \in \mathbb{R}$  and  $[a_x, a_y^\dagger] = [c_x, c_y^\dagger] = \delta(x-y)$ .<sup>2</sup> If we now parameterise  $r(x)$  by introducing a new function  $\xi(x)$  through  $r(x) = \ln \xi(x)$  where  $\xi(x) \in [0, +\infty)$  using Eq. (127) and (128) we find after renormalising

$$\begin{aligned} \int_{x_{min}}^{x_{max}} dx g(x) a_x^\dagger a_x &= \int_{x_{min}}^{x_{max}} dx \frac{g(x)}{4\xi^2(x)} \left( (\xi^4(x) - 1)(e^{i\Delta\theta(x)} c_x^\dagger c_x^\dagger + e^{-i\Delta\theta(x)} c_x c_x) \right. \\ &\quad \left. + 2(\xi^4(x) + 1) c_x^\dagger c_x \right) \end{aligned} \quad (129)$$

where  $\Delta\theta(x) = \theta_2(x) - \theta_1(x)$ . We note that as far as Eq. (129) is concerned, we can set  $\theta_1(x) = -\theta_2(x)$  without losing any generality. With this definition of  $\theta_1(x)$ , the system-environment term simplifies to

$$\hat{A} \int_{x_{min}}^{x_{max}} dx h(x) (a_x + a_x^\dagger) = \hat{A} \int_{x_{min}}^{x_{max}} dx h(x) \xi(x) (e^{i\theta_2(x)} c_x^\dagger + e^{-i\theta_2(x)} c_x). \quad (130)$$

For appropriate choice of the function  $\xi(x)$ , we can define a measure

$$d\lambda(x) = M(x)dx \quad (131)$$

$$M(x) = h^2(x)\xi^2(x). \quad (132)$$

This measure allows us to define a set of monic polynomials  $\{\pi_n(d\lambda; x)\}_{n=0}^\infty$ , which we can use to define the set of functions  $\{U_n(d\lambda; x)\}_{n=0}^\infty$  through the relation

$$U_n(d\lambda; x) = \frac{\pi_n(d\lambda; x) \sqrt{M(x)}}{\sqrt{\langle \pi_n(d\lambda), \pi_n(d\lambda) \rangle_M}} = \frac{\pi_n(d\lambda; x) h(x) \xi(x)}{\sqrt{\langle \pi_n(d\lambda), \pi_n(d\lambda) \rangle_M}}. \quad (133)$$

We can now define the set of creation and annihilation operators of the chain

$$b_n^\dagger = \int_{x_{min}}^{x_{max}} dx U_n(d\lambda; x) c_x^\dagger, \quad (134)$$

$$b_n = \int_{x_{min}}^{x_{max}} dx U_n(d\lambda; x) c_x, \quad (135)$$

with inverse relation

$$c_x^\dagger = \sum_{n=0}^{\infty} U_n(d\lambda; x) b_n^\dagger, \quad (136)$$

$$c_x = \sum_{n=0}^{\infty} U_n(d\lambda; x) b_n. \quad (137)$$

---

<sup>2</sup> We can replace the *cosh* and *sinh* functions with *cos* and *sin* functions for fermions.

Let us now assume that the phase factors are constant<sup>3</sup>  $\theta_2(x) = A_2 = \text{constant}$ . After substitution of Eq. (136) and Eq. (137) into Eq. (130) we obtain

$$\hat{A} \int_{x_{min}}^{x_{max}} dx h(x) (a_x + a_x^\dagger) = \sqrt{\beta_0(d\lambda)} \hat{A} (e^{iA_2} b_0^\dagger + e^{-iA_2} b_0). \quad (138)$$

So we note that for all functions  $\xi(x)$  that result in a valid measure Eq. (131), one can achieve a coupling between system and reservoir which only interacts with the first element in the chain.

Now we will examine carefully what type of chain can be generated via this generalised mapping.

Using the orthogonality conditions of the orthogonal polynomials and Eq. (136) and (137), we can transform terms of the form  $\int_{x_{min}}^{x_{max}} c_{ax} c_{bx} dx$  into terms of the form  $\sum_{n=0}^{\infty} W_n b_{an} b_{bn}$  where the  $W_n$ 's are constants and the sub indices  $a, b = 0$  denote that the operator is an annihilation operator and  $a, b = 1$  denote that they are creation operators. Also, we can transform terms of the form  $\int_{x_{min}}^{x_{max}} x c_{ax} c_{bx} dx$  into  $\sum_{n=0}^{\infty} W_n b_{an} b_{bn} + W_1 b_{a(n+1)} b_{bn} + W_{2n} b_{an} b_{b(n+1)}$  by using the three term recurrence relations Eq. (5) to eliminate the  $x$ . We can also map terms of the form  $\int_{x_{min}}^{x_{max}} x^k c_{ax} c_{bx} dx$   $k = 2, 3, 4, \dots$  using the three term recurrence relations  $k$  times, but this would result in every chain site coupling to its  $k$ th nearest neighbours.<sup>4</sup> Given this reasoning, we speculate that there is only one trial solution to Eq. (129) using real polynomials with  $\Delta\theta(x) = 2\theta_2(x) = 2A_2$  which will map it onto a chain of nearest neighbour interactions. This is:

$$\frac{g(x)}{4\xi^2(x)} (\xi^4(x) - 1) = c_1 + g_1 x, \quad (139)$$

$$\frac{g(x)}{2\xi^2(x)} (\xi^4(x) + 1) = c_2 + g_2 x. \quad (140)$$

Solving these gives us

$$\xi(x) = \left[ \frac{(c_2 + 2c_1) + (g_2 + 2g_1)x}{(c_2 - 2c_1) + (g_2 - 2g_1)x} \right]^{1/4}, \quad (141)$$

$$g(x) = \sqrt{[(c_2 - 2c_1) + (g_2 - 2g_1)x][(c_2 + 2c_1) + (g_2 + 2g_1)x]}. \quad (142)$$

We will now work out the corresponding measure. Using the formula for the differentiation of an inverse function,

$$\left[ \frac{dg^{-1}(x)}{dx} \right] (x) = 1 / \left[ \frac{dg(x)}{dx} \right] (g^{-1}(x)) \quad (143)$$

and Eq. (118), we find

$$h^2(x) = \frac{J(g(x))}{\pi} \left[ \frac{dg(x)}{dx} \right] (x), \quad (144)$$

<sup>3</sup> If we were using complex polynomials, we could leave it as a function of  $x$  and hence we would have to impose a less restrictive constraint. See footnote (6).

<sup>4</sup> We could also transform terms of the form  $\int_{x_{min}}^{x_{max}} f(x) c_{ax} c_{bx} dx$  using orthogonal polynomials in  $f(x)$ , but this will result in the same chain mapping if we choose  $f(x) = x$  and using the standard orthogonal polynomials in  $x$ , so we will stick with the simple  $x$  case only.

so using Eq. (131), we have that the measure  $M(x)$  is

$$M(x) = h^2(x)\xi^2(x) = \frac{J(g(x))}{\pi} \left[ \frac{dg(x)}{dx} \right] (x)\xi^2(x). \quad (145)$$

Let us define a particular relation between the independent variables  $c_1, c_2, g_1, g_2$ , namely

$$2g_1 = q g_2, \quad (146)$$

$$2c_1 = -q c_2, \quad (147)$$

where  $q \in [0, 1]$ .<sup>5</sup> We now find using Eq. (141), (142), and (145)

$$\xi(x) = \left[ \frac{(1-q)c_2 + (1+q)g_2x}{(1+q)c_2 + (1-q)g_2x} \right]^{1/4}, \quad (148)$$

$$g(x) = \sqrt{[(1+q)c_2 + (1-q)g_2x][(1-q)c_2 + (1+q)g_2x]}, \quad (149)$$

$$M(x) = J(g(x)) \frac{g_2}{\pi} \frac{(1+q^2)c_2 + (1-q^2)g_2x}{(1+q)c_2 + (1-q)g_2x}. \quad (150)$$

For convenience, we will denote the quantities in Eq. (148), (149) and (150) by

$$\xi^q(g_2x) = \xi(x), \quad (151)$$

$$g^q(g_2x) = g(x), \quad (152)$$

$$g_2M^q(g_2x) = M(x), \quad (153)$$

where  $\xi^q(x)$ ,  $g^q(x)$  and  $M^q(x)$  are independent of  $g_2$ , to remind us of their  $q$  and  $g_2$  dependency. We will also denote

$$d\lambda^q = g_2M^q(g_2x)dx, \quad (154)$$

$$\alpha_n(q) = \alpha_n(d\lambda^q), \quad (155)$$

$$\beta_n(q) = \beta_n(d\lambda^q). \quad (156)$$

First we note from definition (16) that the support of  $M^q(x)$  is determined by the domain of  $J(x)$ . As we have chosen the domain of  $J(x)$  to be  $[0, \omega_{max}]$ , we need to choose the support of  $g_2M^q(g_2x)$  such that the  $J(x)$  is integrated over its full domain. By observing Eq. (150), we see that we need to choose  $x_{min}$  such that  $g^q(x_{min}) = 0$ . There are two such values which satisfy this requirement,

$$x_{min\pm} = -(c_2/g_2)(1 \pm q)/(1 \mp q). \quad (157)$$

We will take  $x_{min-}$  as it does not contain any singularities in  $q$ . Furthermore, we will set  $c_2 = q/4$  as this will allow us to compare the extremal solutions of the mapping easily as we will see later. We note that for  $g_2 > 0$  the measure has no singularities for well defined spectral densities  $J(x)$ . Also  $\xi^q(x)$  and  $g^q(x)$  are positive functions in their domain  $[x_{min-}, x_{max}]$  for all  $x_{max} > x_{min-}$ . Furthermore, the measure  $d\lambda^q$  satisfies the requirements

---

<sup>5</sup> In principle there are other choices for these constants which will result in other types of coupling relations between the chain elements. We have chosen this particular case as it will result in a particularly interesting solution.

of definition (1) and hence it is a valid measure. We can also find a value for  $x_{max}$ . By observing Eq. (150) we see that we need  $x_{max}$  to satisfy  $g^q(g_2 x_{max}) = \omega_{max}$ . There is only one solution to this which satisfies  $x_{max} > x_{min-}$  which is

$$x_{max} = \left( q(q^2 + 1) - 2\sqrt{q^4 - 4\omega_{max}^2(q^2 - 1)} \right) / (4g_2(q^2 - 1)). \quad (158)$$

For now on we will write  $x_{min-} = x_{min-}(q)$  and  $x_{max} = x_{max}(q)$  to remind us of the  $q$  dependency. The transformation is now well defined with no degrees of freedom other than  $q$  and  $g_2$ .

Now let us perform the mapping. After substituting Eq. (136) and (137), into Eq. (129) and using the orthogonality conditions, we find<sup>6</sup>

$$\int_{x_{min-}(q)}^{x_{max}(q)} dx g_2 g^q(g_2 x) a_x^\dagger a_x \quad (159)$$

$$= \sum_{n=0}^{\infty} \left\{ \left( \frac{q g_2}{2} \alpha_n(q) - \frac{q^2}{8} \right) (e^{2iA_2} b_n^\dagger b_n^\dagger + e^{-2iA_2} b_n b_n) + \left( g_2 \alpha_n(q) + \frac{q}{4} \right) b_n^\dagger b_n \right. \quad (160)$$

$$\left. + g_2 \sqrt{\beta_{n+1}(q)} \left( q(e^{2iA_2} b_n^\dagger b_{n+1}^\dagger + e^{-2iA_2} b_n b_{n+1}) + (b_n^\dagger b_{n+1} + b_n b_{n+1}^\dagger) \right) \right\}. \quad (161)$$

□

*Remark 3* Note that in the generalised mapping, theorem (16), the spectral density can represent continuous modes and/or discrete modes. The discrete modes are represented by dirac delta distributions and the continuous modes by continuous functions. In the case of  $N$  discrete modes only, the generalised mapping will map the system onto a chain with  $N$  sites. Mathematically, the reason for this is because the inner product of the measure (2) in this case can only be defined for functions living in the space spanned by a set of  $N$  orthogonal polynomials of finite degree (See *discrete measure*, page 4 following Theorem 1.8 of [27]). Physically, this is because the number of degrees of freedom corresponding to the Hamiltonian after and before the mapping have to be the same. Also see remark (6) regarding other features of spectral densities.

In addition, it is also worth noting that if the system interacts linearly with more than one environment through different system operators  $\hat{A}$  for each environment, then one can easily generalise the results of the generalised mapping (theorem (16)) such that we can map the Hamiltonian onto a Hamiltonian where the system interacts with more than one chain (i.e. one chain for each environment).

**Lemma 10** *Without loss of generality, we can set  $g_2 = 1$  in theorem (16).*

<sup>6</sup> We note that in order to perform the mapping, we have had to set the phase factors of the Bogoliubov transformation  $\theta_1(x)$  and  $\theta_2(x)$  equal to constants. From (159) we see that this restriction means that they play the simple role of a change of phase of the new variables  $b_n$  and  $b_n^\dagger$ . If one were to work with complex polynomials, one could have probably imposed less stringent constraints and then the phase factors would play a more interesting role such as a gauge transformation.

*Proof* First we will denote  $d\lambda^q(x) = d\lambda^q(g_2, x)$  to make explicit their  $g_2$  dependency. From definition (2), we have that the induced norm of the monic polynomials  $\{\pi_n(d\lambda^q(g_2); x)\}_{n=0}^\infty$  is generated by the inner product

$$\langle \pi_n(d\lambda^q(g_2); x), \pi_n(d\lambda^q(g_2); x) \rangle_{d\lambda^q(g_2)} \quad n = 0, 1, 2, \dots \quad (162)$$

By making the change of variable  $y = x/g_2$ , we can write this as

$$\langle \pi_n(d\lambda^q(g_2); x), \pi_n(d\lambda^q(g_2); x) \rangle_{d\lambda^q(g_2)} = \langle \pi_n(d\lambda^q(1); g_2 y), \pi_n(d\lambda^q(1); g_2 y) \rangle_{d\lambda^q(1)} \quad (163)$$

$n = 0, 1, 2, \dots$ . However we note that this change of variable means that the polynomials  $\pi_n(d\lambda^q(1); g_2 y)$   $n = 0, 1, 2$  in the RHS of Eq. (163) are monic polynomials in  $g_2 y$  and hence are not monic polynomials for measure  $d\lambda^q(1, y)$ . To make them monic polynomials in  $y$ , we must make their leading coefficient unity. Hence by dividing both sides of Eq. (163) by  $g_2^{2n}$  we get the relation

$$\langle \pi_n(d\lambda^q(1); y), \pi_n(d\lambda^q(1); y) \rangle_{d\lambda^q(1)} = \frac{\langle \pi_n(d\lambda^q(g_2); x), \pi_n(d\lambda^q(g_2); x) \rangle_{d\lambda^q(g_2)}}{g_2^{2n}} \quad (164)$$

$n = 0, 1, 2, \dots$ . Similarly, we find

$$\langle y \pi_n(d\lambda^q(1); y), \pi_n(d\lambda^q(1); y) \rangle_{d\lambda^q(1)} = \frac{\langle x \pi_n(d\lambda^q(g_2); x), \pi_n(d\lambda^q(g_2); x) \rangle_{d\lambda^q(g_2)}}{g_2^{2n+1}} \quad (165)$$

$n = 0, 1, 2, \dots$ . Hence using Eq. (164) and (165) together with Eq. (7), (8) (9) we find

$$\sqrt{\beta_0(d\lambda^q(1))} = \sqrt{\beta_0(d\lambda^q(g_2))}, \quad (166)$$

$$\sqrt{\beta_n(d\lambda^q(1))} = g_2 \sqrt{\beta_n(d\lambda^q(g_2))} \quad n = 1, 2, 3, \dots, \quad (167)$$

$$\alpha_n(d\lambda^q(1)) = g_2 \alpha_n(d\lambda^q(g_2)) \quad n = 1, 2, 3, \dots \quad (168)$$

Hence by comparing Eq. (166), (167) and (168) with the chain coefficients in Eq. (138) and Eq. (159), we see that the chain mapping coefficients are invariant under any choice of  $g_2 > 0$ .  $\square$

**Corollary 4** *The generalised mapping Eq. (122) reduces to*

$$H \mapsto H_S + \sqrt{\beta_0(0)} A(b_0 + b_0^\dagger) + \sum_{n=0}^{\infty} g_2 \alpha_n(0) b_n^\dagger b_n + g_2 \sqrt{\beta_{n+1}(0)} (b_{n+1}^\dagger b_n + h.c.). \quad (169)$$

when  $q = 0$ ,  $A_2 = 0$ . We also find

$$M^0(x) = \frac{J(x)}{\pi}, \quad (170)$$

$$g^0(x) = x, \quad (171)$$

$$\{x_{min}(0), x_{max}(0)\} = \{0, \omega_{max}/g_2\}. \quad (172)$$

*This is just the known result of* found in [19] and [18].

*Proof* Follows from setting  $q = 0$ ,  $A_2 = 0$  in theorem (16) and simplifying the resultant expressions.  $\square$

Given that the coupling of the chain elements is excitation number preserving, the elementary excitations of the chain can be viewed as particles hopping on a 1d lattice. We therefore make the following definition.

**Definition 17** *We shall refer to the transformation described in corollary (4) as the particle mapping.*

*Remark 4* lemma (10) clarifies the role of the constant  $g$  in [18] as the  $g_2$  constant defined in this article is equivalent to the  $g$  constant in their article for the particle mapping.

**Corollary 5** *When  $q = 1$ ,  $A_2 = 0$ , the generalised mapping Eq. (122) reduces to*

$$H \rightarrow H_S + \sqrt{\beta_0(1)}\hat{A}X_0 + \sum_{n=0}^{\infty} \left( g_2 \sqrt{\beta_{n+1}(1)} X_n X_{n+1} + g_2 \frac{\alpha_n(1)}{2} X_n^2 + \frac{1}{2} P_n^2 \right). \quad (173)$$

where  $X_n$  and  $P_n$  are position and momentum operators,  $X_n := (b_n^\dagger + b_n)$ ,  $P_n := i(b_n^\dagger - b_n)/2$   $n = 0, 1, 2, \dots$ . We also find

$$g^1(x) = \sqrt{x}, \quad (174)$$

$$M^1(x) = \frac{J(\sqrt{x})}{\pi}, \quad (175)$$

$$\{x_{\min}(1), x_{\max}(1)\} = \{0, \omega_{\max}^2/g_2\}. \quad (176)$$

*Proof* Follows from setting  $q = 1$ ,  $A_2 = 0$  in theorem (16) and simplifying the resultant expressions.  $\square$

Given that the coupling of the chain elements in Eq. (173) resemble that of springs obeying Hooke's law, the elementary excitations are phonons such as in solid state physics. We therefore make the following definition.

**Definition 18** *We shall refer to the transformation described in corollary (5) as the phonon mapping.*

*Remark 5* In light of definitions (17) and (18), we note that Eq. (122) interpolates between the two solutions.

**Definition 19** *We call  $m$ th embedding to the new system-environment interaction produced when the new system is composed of the initial system plus the first  $m$  sites of the chain formed by the environment in the chain representation. The new environment is formed by the remaining chain elements. See figure (c).*

As we will see in section 3.4, the chain coefficients converge for a wide range of spectral densities, and hence all the specific features of an environment appear in the first sites of the chain. Consequentially, these can be progressively (or directly, all in one go) absorbed into the system by making an embedding; to reduce the complexity of the effective environment.



**Corollary 6** *The generalised mapping in terms of Jacobi matrices is:*

$$H = H_S + \sqrt{\beta_0(q)} \hat{A}(e^{iA_2} b_0^\dagger + e^{-iA_2} b_0) \quad (177)$$

$$+ \frac{q}{2} \left[ e^{-2iA_2} \mathbf{b}_0^T \left( \mathcal{J}(d\lambda^q) - \frac{q}{4} \mathbb{I} \right) \mathbf{b}_0 + h.c. \right] + \mathbf{b}_0^\dagger \left( \mathcal{J}(d\lambda^q) + \frac{q}{4} \mathbb{I} \right) \mathbf{b}_0,$$

where

$$\mathbf{b}_n := (b_n, b_{n+1}, b_{n+2}, b_{n+3}, \dots)^T, \quad n = 0, 1, 2, \dots, \quad (178)$$

and  $\dagger$  is understood as the transpose plus h.c. of the elements of the vector. After the  $m$ th embedding the Hamiltonian is

$$H = H_{S_m^q} + g_2 \sqrt{\beta_m(q)} \left( q(e^{2iA_2} b_{m-1}^\dagger b_m^\dagger + e^{-2iA_2} b_{m-1} b_m) + (b_{m-1}^\dagger b_m + b_{m-1} b_m^\dagger) \right) \quad (179)$$

$$+ \frac{q}{2} \left[ e^{-2iA_2} \mathbf{b}_m^T \left( \mathcal{J}_m(d\lambda^q) - \frac{q}{4} \mathbb{I} \right) \mathbf{b}_m + h.c. \right] + \mathbf{b}_m^\dagger \left( \mathcal{J}_m(d\lambda^q) + \frac{q}{4} \mathbb{I} \right) \mathbf{b}_m \quad (180)$$

$$m = 1, 2, 3, \dots,$$

where the Hamiltonian of the system part of the  $m$ th embedding,  $H_{S_m^q}$  is given by

$$H_{S_m^q} := H_S + \sqrt{\beta_0(q)} \hat{A}(e^{iA_2} b_0^\dagger + e^{-iA_2} b_0) \quad (181)$$

$$+ \sum_{n=0}^{m-2} \sqrt{\beta_{n+1}(q)} \left( q(e^{2iA_2} b_n^\dagger b_{n+1}^\dagger + e^{-2iA_2} b_n b_{n+1}) + (b_n^\dagger b_{n+1} + b_n b_{n+1}^\dagger) \right) \quad (182)$$

$$+ \sum_{n=0}^{m-1} \left( \frac{q}{2} \alpha_n(q) - \frac{q^2}{8} \right) (e^{2iA_2} b_n^\dagger b_n^\dagger + e^{-2iA_2} b_n b_n) + \left( \alpha_n(q) + \frac{q}{4} \right) b_n^\dagger b_n. \quad (183)$$

For the particular cases of the particle and phonon mappings, this reduces to

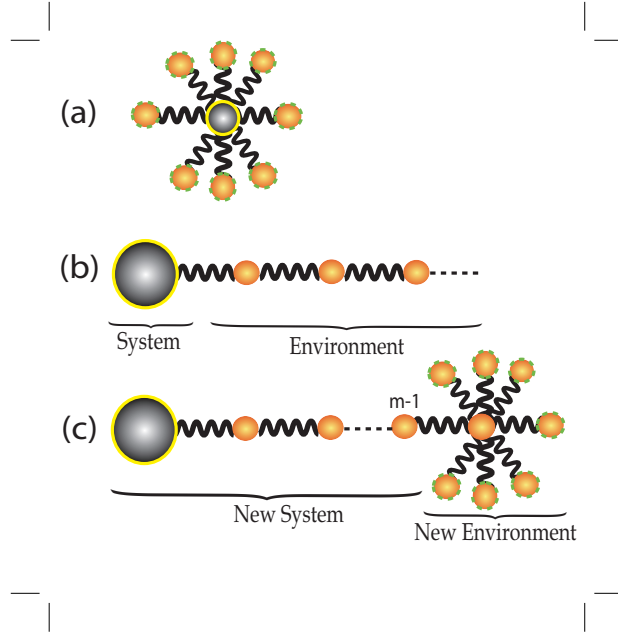
$$H = H_{S_m^0} + \sqrt{\beta_m(d\lambda^0)} (b_m^\dagger b_{m-1} + h.c.) + \mathbf{b}_m^\dagger \mathcal{J}_m(d\lambda^0) \mathbf{b}_m \quad m = 1, 2, 3, \dots, \quad (184)$$

$$H = H_{S_m^1} + \sqrt{\beta_m(d\lambda^1)} X_m X_{m-1} + \frac{1}{2} \mathbf{X}_m^T \mathcal{J}_m(d\lambda^1) \mathbf{X}_m + \frac{1}{2} \mathbf{P}_m^T \mathbf{P}_m \quad (185)$$

$m = 1, 2, 3, \dots$ , respectively. Where  $\mathbf{X}_n := (X_n, X_{n+1}, X_{n+2}, \dots)^T$ ,  $\mathbf{P}_n := (P_n, P_{n+1}, P_{n+2}, \dots)^T$ ,  $n = 0, 1, 2, \dots$ .

*Proof* Eq. (177) follows from writing Eq. (159) in terms of the Jacobi matrix of the measure  $d\lambda^q$  and Eq. (179) then follows using the identity  $\mathcal{J}(d\lambda_m^q) = \mathcal{J}_m(d\lambda^q)$  which is a direct consequence of corollary (3).  $\square$

**Definition 20** *We call the  $n$ th partial spectral density  $J_n(\omega)$  to the spectral density which describes the system-environment interaction of the  $n$ th embedding. We call the initial spectral density  $J_0(\omega)$  such that  $J_0(\omega) \equiv J(\omega)$ . See figure (c).*



**Fig. 1** (a) The initial system-environment Hamiltonian before the mapping has been performed: the system (depicted by the gray ball in the centre) couples directly to the degrees of freedom of the environment (orange balls). (b) The system-environment Hamiltonian after the chain mapping has been performed: the environment has been mapped onto a semi-infinite chain of nearest neighbour interactions where the system now only couples to the first element in the chain. (c) The system-environment Hamiltonian after the  $m$ th environmental degree of freedom has been embedded: the new system, interacts with the new environment via the  $m$ th partial spectral density  $J_m(x)$ .

### 3.2 Connection between the phonon mapping to previous work and the sequence of partial spectral densities

**Theorem 17** *The sequence of partial spectral densities in [21] are generated by*

$$J_n(\omega) = \frac{J_0(\omega)}{(P_{n-1}(d\lambda^1; \omega^2) \frac{\varphi(d\lambda^1; \omega^2)}{2} - Q_{n-1}(d\lambda^1; \omega^2))^2 + J_0^2(\omega) P_{n-1}^2(d\lambda^1; \omega^2)} \quad (186)$$

$n = 1, 2, 3, \dots$ , where  $g_2 = 1$ .

*Proof* As observed by Leggett [35], the spectral density of an open quantum system can be easily obtained from its propagator  $L_0(z)$ . The authors of [21] have developed this to find a continued fraction representation for the case of the mapping of the propagator presented in their paper as follows.

$$L_0(z) = -z^2 - w_0(z), \quad (187)$$

$$w_0(z) = \frac{D_0^2}{\Omega_1^2 - z^2 - \frac{D_1^2}{\Omega_2^2 - z^2 - \frac{D_2^2}{\Omega_3^2 - z^2 - \dots}}}, \quad (188)$$

where

$$D_n^2 = \frac{2}{\pi} \int_0^\infty d\omega J_n(\omega) \omega \quad n = 0, 1, 2, \dots, \quad (189)$$

$$\Omega_{n+1}^2 = \frac{2}{\pi D_n^2} \int_0^\infty d\omega J_n(\omega) \omega^3 \quad n = 0, 1, 2, \dots. \quad (190)$$

Alternatively, we note that we can write the continued fraction Eq. (188) as a recurrence relation

$$w'_n(\sqrt{z}) = \frac{D_n^2}{z - \Omega_{n+1}^2 - w'_{n+1}(\sqrt{z})} \quad n = 0, 1, 2, \dots, \quad (191)$$

where  $w'_n(z) := -w_n(z)$ . From [21], we have an alternative expression for  $w_n$  in terms of the partial spectral densities through the relation,

$$w_n(z) = \frac{2}{\pi} \int_0^\infty d\omega \frac{J_n(\omega) \omega}{\omega^2 - z^2} \quad n = 0, 1, 2, \dots, \quad (192)$$

which by a change of variables and taking into account the definition of  $\omega'_n$  in Eq. (191), can be written in the form

$$w'_n(\sqrt{z}) = \frac{1}{\pi} \int_0^\infty d\omega \frac{J_n(\sqrt{\omega})}{z - \omega} \quad n = 0, 1, 2, \dots. \quad (193)$$

Furthermore, via a change of variables the integrals Eq. (189) and (190) can be written as

$$D_n^2 = \frac{1}{\pi} \int_0^\infty d\omega J_n(\sqrt{\omega}) \quad n = 0, 1, 2, \dots, \quad (194)$$

$$\Omega_{n+1}^2 = \frac{1}{\pi D_n^2} \int_0^\infty d\omega J_n(\sqrt{\omega}) \omega \quad n = 0, 1, 2, \dots. \quad (195)$$

We note that in [21] the support of the spectral densities corresponds with the domain of the spectral densities defined in definition (16) and hence integrals Eq. (193), (194) and (195) are zero outside of the domain of  $J_n(x)$ ,  $n = 0, 1, 2, \dots$ , therefore we can change the upper infinity limit of the integrals by  $\omega_{max}^2$ . Now let us define the set of measures

$$d\gamma_n(t) = dt \bar{\gamma}_n(t) \quad n = 0, 1, 2, \dots, \quad (196)$$

$$\bar{\gamma}_n(t) = \frac{J_n(\sqrt{t})}{\pi D_n^2} \quad n = 0, 1, 2, \dots. \quad (197)$$

This definition of the measure has some important consequences:

- 1) From Eq. (195) we note that  $\Omega_{n+1}^2$  are the first moments of the measures  $d\gamma_n(t)$ ,

$$C_1(d\gamma_n) = \Omega_{n+1}^2 \quad n = 0, 1, 2, \dots. \quad (198)$$

- 2) From Eq. (193) and definition (7) we see that  $w'_n(\sqrt{z})$  is proportional to the Stieltjes transformations of the measure  $d\gamma_n(t)$

$$w'_n(\sqrt{z}) = D_n^2 S_n(z) \quad n = 0, 1, 2, \dots. \quad (199)$$

3) From Eq. (194) we see that the zeroth moments of the measures  $d\gamma_n(t)$  are unity

$$C_0(d\gamma_n) = 1 \quad n = 0, 1, 2, \dots \quad (200)$$

We are now able to re-write Eq. (191) in the form

$$S_{n+1}(z)D_{n+1}^2 = z - C_1(d\gamma_n) - \frac{1}{S_n(z)}, \quad n = 0, 1, 2, \dots, \quad (201)$$

where we have used the short hand  $S_{m_n}(z) =: S_n(z)$ . By comparing this recursion relation with Eq. (19) and definition (8), we deduce that  $D_{n+1}^2 d\gamma_{n+1}$  is the secondary measure associated with  $d\gamma_n$ , for  $n = 0, 1, 2, \dots$ . We can also identify a sequence of normalised secondary measures. Noting that  $C_0(d\gamma_0) = 1$  from Eq. (200), definition (9) tells us that the sequence of secondary normalised measures starting from  $d\gamma_0$  is

$$d\gamma_0, D_1^2 d\gamma_1 / C_0(D_1^2 d\gamma_1), D_2^2 d\gamma_2 / C_0(D_2^2 d\gamma_2), \dots, D_m^2 d\gamma_m / C_0(D_m^2 d\gamma_m), \dots \quad (202)$$

However,

$$C_0(D_n^2 d\gamma_n) = D_n^2 C_0(d\gamma_n) = D_n^2 \quad n = 1, 2, 3, \dots, \quad (203)$$

so the sequence of normalised secondary measures is  $d\gamma_0(t), d\gamma_1(t), d\gamma_2(t), d\gamma_3(t), \dots$ . Taking into account lemma (3) and theorem (8) we see that

$$D_n^2 = d_{n-1} = \beta_n(d\gamma_0) \quad n = 1, 2, 3, \dots \quad (204)$$

Due to corollary (1) and Eq. (200) we can also write  $D_0^2$  in terms of  $\beta_0$ ,

$$D_0^2 = \beta_0(d\eta_0) \quad (205)$$

where

$$d\eta_0 := D_0^2 d\gamma_0. \quad (206)$$

We can now construct a sequence of beta normalised measures from  $d\eta_0$ , denoted by  $d\eta_0, d\eta_1, d\eta_2, \dots$ . From Eq. (205) and (206) we see that  $d\eta_0$  satisfies Eq. (101) for  $d\gamma_0$ , hence lemma (9) tells us

$$\bar{\eta}_n(x) = \beta_n(d\eta_0) \bar{\gamma}_n(x) \quad n = 0, 1, 2, \dots \quad (207)$$

Taking into account that  $\beta_n(d\eta_0) = \beta_n(d\gamma_0)$   $n = 1, 2, 3, \dots$  due to lemma (7) and Eq. (206), from Eq. (207) and (197) we gather

$$d\eta_n(t) = dt \bar{\eta}_n(t) \quad n = 0, 1, 2, \dots, \quad (208)$$

$$\bar{\eta}_n(t) = \frac{J_n(\sqrt{t})}{\pi} \quad n = 0, 1, 2, \dots, \quad (209)$$

hence we note that

$$d\eta_0 = d\lambda^1. \quad (210)$$

Substituting this into Eq. (99) gives us Eq. (186).  $\square$

**Theorem 18** *The mapping described in [21] is a special case of the generalised mapping, theorem (16), namely it is equivalent to the phonon mapping.*

*Proof* The mapping in [21] is

$$H \rightarrow H_S - D_0 s X_1 + \sum_{n=1}^{\infty} \left( -D_n X_n X_{n+1} + \frac{\Omega_n^2}{2} X_n^2 + \frac{1}{2} P_n^2 \right), \quad (211)$$

where  $H_S = \frac{P^2}{2m} + V(s) + \Delta V(s)$ . See [21] for full details. From Eq. (195) and (7) we see that we can write  $\Omega_n^2$  as

$$\Omega_{n+1}^2 = \alpha_0(d\eta_n) \quad n = 0, 1, 2, \dots \quad (212)$$

Hence,

$$\Omega_{n+1}^2 = \alpha_n(d\eta_0) = \alpha_n(d\lambda^1) = \alpha_n(1) \quad n = 0, 1, 2, \dots, \quad (213)$$

where we have used Eq. (108) followed by Eq. (210) and (155). From Eq. (194), and (9) we see that

$$D_n^2 = \beta_0(d\eta_n) \quad n = 0, 1, 2, \dots \quad (214)$$

Hence using Eq. (109) followed by Eq. (210) and (155), we find

$$D_n^2 = \beta_n(d\eta_0) = \beta_n(d\lambda^1) = \beta_n(1) \quad n = 0, 1, 2, \dots \quad (215)$$

If we let  $A = s$  in Eq. (173) and make the change of variable  $n \rightarrow n+1$  in the summation and relabel the position momentum variables such that  $(X_n, P_n) \rightarrow (X_{n+1}, P_{n+1}) \quad n = 0, 1, 2, \dots$ , from Eq. (213) and (215) we find

$$H \rightarrow H_S + D_0 s X_1 + \sum_{n=1}^{\infty} \left( D_n X_n X_{n+1} + \frac{\Omega_n^2}{2} X_n^2 + \frac{1}{2} P_n^2 \right). \quad (216)$$

Now if we redefine the position and momentum variables by performing a phase rotation  $X_n \rightarrow X_n(-1)^n$ ,  $P_n \rightarrow P_n(-1)^n$  to get a minus sign in the interaction terms and let  $H_S = \frac{P^2}{2m} + V(s) + \Delta V(s)$  in Eq. (173), we find Eq. (211).  $\square$

*Remark 6* We note that the three term recurrence relations Eq. (5) for measures with gaps (i.e. measures  $d\mu(x) = \bar{\mu}(x)dx$  where the support of  $\bar{\mu}(x)$  is not one section of the real line, but rather has disjointed support regions i.e.  $I = [a, b] \cup [c, d]$  where  $b < c$ ), still hold. Hence the generalised mapping (and therefore the phonon mapping) is still valid. However, the chain mapping presented in [21] is not valid under these conditions because the Stieltjes transformation of a measure, definition (7) is not valid anymore and hence one cannot calculate the chain coefficients from the sequence of partial spectral densities. In this sense, the phonon mapping presented here is a more general result. This is an important difference because if a spectral density has a gap in its support, then the corresponding measure also has a gap. There are physical systems (such as photonic crystals and diatomic chains) which have these properties.

**Corollary 7** *In the phonon mapping case, the sequence of partial spectral densities is given by*

$$J_n(\omega) = \frac{J_0(\omega)}{(P_{n-1}(d\lambda^1; \omega^2) \frac{\varphi(d\lambda^1; \omega^2)}{2} - Q_{n-1}(d\lambda^1; \omega^2))^2 + J_0^2(\omega) P_{n-1}^2(d\lambda^1; \omega^2)} \quad (217)$$

$n = 1, 2, 3, \dots$ , where  $g_2 = 1$ .

*Proof* Follows directly from theorems (17) and (18). Also see section 6.1 in the appendix.  $\square$

### 3.3 Sequence of partial spectral densities for the particle mapping case

**Theorem 19** *In the particle mapping case, the sequence of partial spectral densities is given by*

$$J_n(\omega) = \frac{J_0(\omega)}{(P_{n-1}(d\lambda^0; \omega) \frac{\varphi(d\lambda^0; \omega)}{2} - Q_{n-1}(d\lambda^0; \omega))^2 + J_0^2(\omega) P_{n-1}^2(d\lambda^0; \omega)} \quad (218)$$

$n = 1, 2, 3, \dots$ , where  $g_2 = 1$ .

*Proof* The proof will start by defining a set of initially independent Hamiltonians. Each one of these will represent some system-environment interaction of a similar type discussed in this paper. When they are in this form, we can easily find an expression for the spectral density representing the system-environment interaction. We then put constraints on the Hamiltonians in such a way that they are no-longer independent from one another. Finally we show that these spectral densities correspond to the sequence of spectral densities for the particle mapping.

Let us start by defining a set of independent Hamiltonians

$$H_m = H_{Sm} + \int_0^{x_{max}(0)} g(x) a_{mx} a_{mx}^\dagger dx + \int_0^{x_{max}(0)} h_m(x) (a_{mx}^\dagger b_{m-1} + a_{mx} b_{m-1}^\dagger) dx \quad (219)$$

$m = 1, 2, 3, \dots$ , where  $[a_{mx}, a_{ny}^\dagger] = \delta_{mn} \delta(x - y)$  and  $[b_{m-1}, b_{n-1}^\dagger] = \delta_{mn}$   $m, n = 1, 2, 3, \dots$ .  $b_{m-1}, b_{m-1}^\dagger$  for the  $m$ th Hamiltonian  $H_m$  belong to the system which has Hamiltonian  $H_{Sm}$ . We note that the  $m$ th hamitonian  $H_m$ , has a spectral density  $J^m(x)$  given by<sup>7</sup> Eq. (118):

$$J^m(\omega) = \pi h_m^2 [g^{-1}(\omega)] \frac{dg^{-1}(\omega)}{d\omega}. \quad (220)$$

Now let us set  $g(x) = g_2 x$ . Eq. (220) gives us  $h_m^2(x) = g_2 J^m(g_2 x) / \pi$ . We now define the set of measures

$$d\vartheta_m(x) = h_m^2(x) dx = g_2 J^m(g_2 x) dx / \pi \quad m = 1, 2, 3, \dots, \quad (221)$$

and the new set of creation and annihilation operators through the unitary transformation

$$b_{mn}^\dagger = \int_0^{x_{max}(0)} dx U_n^m(x) a_{mx}^\dagger \quad n = 0, 1, 2, \dots, m = 1, 2, 3, \dots, \quad (222)$$

where  $U_n^m(x) = h_m(x) P_n(d\vartheta_m; x)$   $n = 0, 1, 2, \dots, m = 1, 2, 3, \dots$ . Using the orthogonality conditions of orthonormal polynomials definition (3), we find the inverse relation to be

$$a_{mx}^\dagger = \sum_{n=0}^{\infty} U_n^m(x) b_{mn}^\dagger \quad m = 1, 2, 3, \dots \quad (223)$$

---

<sup>7</sup> We have used a superindex here rather than a subindex to denote the spectral densities so as not to confuse them with partial spectral densities, as at this stage we cannot identify them as such.

Substituting this into the RHS of Eq. (219) and using the three term recurrence relations Eq. (5) and orthogonality conditions Eq. (3), we find that we can write  $H_m$  as

$$H_m = H_{S_m} + \sqrt{\beta_0(d\vartheta_m)}(b_{m0}^\dagger b_{m-1} + b_{m0} b_{m-1}^\dagger) \quad (224)$$

$$+ \sum_{n=0}^{\infty} \sqrt{\beta_{n+1}(d\vartheta_m)}(b_{m(n+1)}^\dagger b_{mn} + h.c.) + \alpha_n(d\vartheta_m) b_{mn}^\dagger b_{mn} \quad (225)$$

$m = 1, 2, 3, \dots$ . We note that at this stage, the set of spectral densities  $\{J^m(x)\}_{m=1}^{\infty}$  are independent and undefined. This freedom allows us to let the set of measures  $\{d\vartheta_m\}_{m=1}^{\infty}$  be a sequence of beta normalised measures generated from the measure  $d\lambda^0$  which from Eq. (154) and (175) we see is given in terms of another spectral density  $J(x)$ . Now the spectral densities  $\{J^m(x)\}_{m=1}^{\infty}$  are fully determined by  $J(x)$  through the definition of a beta normalised sequence of measures, definition (13). Hence using Eq. (99) and (221) we get

$$J^n(\omega) = \frac{J(\omega)}{(P_{n-1}(d\lambda^0; \omega) \frac{\varphi(d\lambda^0; \omega)}{2} - Q_{n-1}(d\lambda^0; \omega))^2 + J^2(\omega) P_{n-1}^2(d\lambda^0; \omega)} \quad (226)$$

$n = 1, 2, 3, \dots$ , where where  $g_2 = 1$ . Now we have to show that  $J^n$  is the  $n$ th partial spectral density for the particle mapping Hamiltonian Eq. (169) i.e. the interaction described by Eq. (184). First let us define  $H_{S_m}$  in Eq. (224) as  $H_{S_m} = H_{S_m^0}$   $m = 1, 2, 3, \dots$  and note that using Eq. (108) and (109), we have

$$\beta_0(d\vartheta_m) = \beta_m(d\lambda^0) \quad m = 1, 2, 3, \dots, \quad (227)$$

$$\alpha_n(d\vartheta_m) = \alpha_{n+m}(d\lambda^0) \quad m = 1, 2, 3, \dots, n = 0, 1, 2, \dots, \quad (228)$$

$$\beta_{n+1}(d\vartheta_m) = \beta_{n+1+m}(d\lambda^0) \quad m = 1, 2, 3, \dots, n = 0, 1, 2, \dots \quad (229)$$

Hence Eq. (224) now becomes

$$H_m = H_{S_m^0} + \sqrt{\beta_m(d\lambda^0)}(b_{m0}^\dagger b_{m-1} + b_{m0} b_{m-1}^\dagger) \quad (230)$$

$$+ \sum_{n=m}^{\infty} \sqrt{\beta_{n+1}(d\lambda^0)}(b_{m(n+1-m)}^\dagger b_{m(n-m)} + h.c.) \quad (231)$$

$$+ \alpha_m(d\lambda^0) b_{m(n-m)}^\dagger b_{m(n-m)} \quad (232)$$

$m = 1, 2, 3, \dots$ , or by writing it in terms of a Jacobi matrix,

$$H_m = H_{S_m^0} + \sqrt{\beta_m(d\lambda^0)}(b_{m0}^\dagger b_{m-1} + h.c.) + \mathbf{b}_{m0}^\dagger \mathcal{J}_m(d\lambda^0) \mathbf{b}_{m0} \quad m = 1, 2, 3, \dots, \quad (233)$$

where  $\mathbf{b}_{m0}^\dagger := (b_{m0}^\dagger, b_{m1}^\dagger, b_{m2}^\dagger, b_{m3}^\dagger, \dots)$ ,  $\mathbf{b}_{m0} := (b_{m0}, b_{m1}, b_{m2}, b_{m3}, \dots)^T$   $m = 1, 2, 3, \dots$ . By comparing Eq. (233) with Eq. (184), we see that we have generated a chain mapping with identical coefficients, hence the spectral densities  $\{J^m(x)\}_{m=1}^{\infty}$  are the partial spectral densities for the particle mapping.  $\square$

### 3.4 Partial spectral densities sequence convergence

**Definition 21** We say that the chain mapping for some  $q$  and a particular spectral density  $J(x)$ , will belong to the Szegő class if the measure  $d\lambda^q(x) = M^q(x)dx$  satisfies

$$\int_{x_{\min-}(q)}^{x_{\max}(q)} \frac{\ln M^q(x) dx}{\sqrt{(x_{\max}(q) - x)(x - x_{\min-}(q))}} > -\infty. \quad (234)$$

*Remark 7* Examples of spectral densities which for any  $q$  do not belong to the Szegő class, are those which have gaps in their domain and those with unbounded support.

**Theorem 20** If for some  $q$ -chain mapping for spectral density  $J(\omega)$  belongs to the Szegő class, then the sequences  $\alpha_0(q), \alpha_1(q), \alpha_2(q), \dots$  and  $\beta_0(q), \beta_1(q), \beta_2(q), \dots$  converge to:

$$\lim_{n \rightarrow \infty} \alpha_n(q) = \frac{x_{\max}(q) + x_{\min-}(q)}{2}, \quad (235)$$

$$\lim_{n \rightarrow \infty} \beta_n(q) = \frac{(x_{\max}(q) - x_{\min-}(q))^2}{16}. \quad (236)$$

*Proof* Follows from shifting the support region of the Szegő theorem in [18]. For the original theorem see [36].  $\square$

**Corollary 8** If for some  $q$ -chain mapping for spectral density  $J(\omega)$  belongs to the Szegő class, the tail of the semi-infinite  $q$ -chain mapping tends to a translational invariant chain.

*Proof* Follows from theorem (20) and Eq. (159).  $\square$

**Definition 22** The moment problem for a measure  $d\mu$  is said to be determined, if it is uniquely determined by its moments.

**Theorem 21** If a measure  $d\mu$  has a finite support interval  $I$ , then its moment problem is determined.

*Proof* See [27].

**Theorem 22** If for some measure  $d\mu(x)$  with finite support interval  $I$  the limits

$$\lim_{n \rightarrow \infty} \alpha_n(d\mu) = \frac{a+b}{2}, \quad (237)$$

$$\lim_{n \rightarrow \infty} \beta_n(d\mu) = \frac{(b-a)^2}{16}, \quad (238)$$

exist, then the sequence of beta normalised and normalised secondary measures generated from  $d\nu$  and  $d\mu$  respectively, converge weakly to

$$\lim_{n \rightarrow \infty} \bar{\nu}_n(x) = \frac{\sqrt{(x-a)(b-x)}}{2\pi}, \quad (239)$$

$$\lim_{n \rightarrow \infty} \bar{\mu}_n(x) = \frac{8\sqrt{(x-a)(b-x)}}{\pi(b-a)^2}. \quad (240)$$

Furthermore, this is the only converging limit which exists.



*Proof* First we will show that the limit exists and is unique by construction, then we will show that it corresponds to when the limits Eq. (237) and (238) are accomplished. Substituting Eq. (60) into Eq. (54), we find

$$\varphi(d\rho; x) = 2[x - C_1(d\mu)] - \frac{\varphi(d\mu; x)\bar{\rho}(x)}{\bar{\mu}(x)}. \quad (241)$$

If the limit exists, then there must be at least one solution to  $\bar{\rho}(x) = A\bar{\mu}(x)$  where  $d\rho(x) = \bar{\rho}(x)dx$  is the secondary measure associated with the measure  $d\mu(x) = \bar{\mu}(x)dx$  and  $A > 0$ . From definitions (11) and (7) we see that  $\varphi(d\rho; x) = A\varphi(d\mu; x)$  and hence from Eq. (241) we see that

$$\varphi(d\mu; x) = \frac{x - C_1(d\mu)}{A}. \quad (242)$$

Thus substituting this into Eq. (54), and solving for  $\bar{\mu}(x)$  we find

$$\bar{\mu}^2(x) = \frac{4A - (x - C_1(d\mu))^2}{4\pi^2 A^2}. \quad (243)$$

Taking into account the definition of a measure, definition (1), we see that if the limit exists, then it must be bounded. Moreover, it must belong to the interval centered at  $C_1(d\mu)$  and of length  $4\sqrt{A}$ . Making the change of variable  $x - C_1(d\mu) = 2\sqrt{A}t$  gives us

$$d\mu(t) = \bar{\mu}(t)dt = \frac{2\sqrt{1-t^2}}{\pi}dt, \quad (244)$$

with support interval  $[-1, 1]$ . We note that at every step of the proof we have used the most general conditions and found the most general solution, hence if this solution exists, it must be unique. We now can check that Eq. (244) exists by direct substitution. Using definition (7) we find that the Stieltjes Transform of Eq. (244) is  $S_{\bar{\mu}}(z) = 2[z - \sqrt{z^2 - 1}]$  and hence from definition (11) we find  $\varphi(d\mu; x) = 4x$ . Thus using Eq. (54) we get  $\bar{\rho}(x) = \bar{\mu}(x)/4$ , hence the limit exists. By performing the change of variable  $t = (2/(b-a))y + (b+a)/(a-b)$ , we shift the support of Eq. (244) to the general case  $[a, b]$  and the measure is now given by Eq. (240).

Now we will proceed to show that if Eq. (237) and (238) are satisfied, then the sequence of normalised secondary measures converge weakly to Eq. (240). By taking the  $n$ th moment of the measures in Eq. (22) and taking into account lemma (24) for  $n = 0$ , we have

$$C_n(d\rho_{n+1}) = [C_2(d\mu_n) - C_1(d\mu_n)^2] C_n(d\mu_{n+1}) \quad n, m = 0, 1, 2, \dots \quad (245)$$

Writing Eq. (24) for a sequence of measures followed by substituting in our expression for  $C_n(d\rho_{n+1})$  using Eq. (245), we find

$$(c_2^s - (c_1^s)^2) c_n^{s+1} = c_{n+2}^s - c_1^s c_{n+1}^s - \sum_{j=0}^{n-1} (c_2^s - (c_1^s)^2) c_j^{s+1} c_{n-j}^s \quad n, s = 0, 1, 2, \dots, \quad (246)$$

where  $c_n^s := C_n(d\mu_s)$   $n, s = 0, 1, 2, \dots$ . Let us define the limit  $l_n = \lim_{s \rightarrow \infty} c_n^s$ . We can now draw the following conclusions

1) Due to corollary (2), we have  $C_0(d\mu_n) = 1$   $n = 0, 1, 2, \dots$ . Therefore  $l_0 = 1$ .

2) From Eq. (87) and (7) we see that

$$\alpha_n(d\mu_0) = \alpha_0(d\mu_n) = \frac{C_1(d\mu_n)}{C_0(d\mu_n)} = c_1^n. \quad (247)$$

Hence taking into account assumption Eq. (237), we have  $l_1 = (a + b)/2$ .

3) Noting the definition of  $d_n$  in theorem (3), theorem (8) tells us

$$\beta_{n+1}(d\mu_0) = c_2^n - (c_1^n)^2 \quad n = 0, 1, 2, \dots \quad (248)$$

Hence taking into account assumptions Eq. (237) and (238), and Eq. (247) we have  $l_2 = (5a^2 + 6ab + 5b^2)/16$ .

We note that for any  $s$ , all the moments  $c_n^s$  in Eq. (246) are fully determined by the starting values  $c_0^s$ ,  $c_1^s$ , and  $c_2^s$ , hence we conclude from the above points 1), 2) and 3), that under the assumptions Eq. (237) and (238), all  $l_n \quad n = 0, 1, 2, \dots$  are finite and determined by

$$(l_2 - l_1^2) l_n = l_{n+2} - l_1 l_{n+1} - (l_2 - l_1^2) \sum_{j=0}^{n-1} l_j l_{n-j} \quad n, s = 0, 1, 2, \dots, \quad (249)$$

with starting values  $l_0 = 1$ ,  $l_1 = (a + b)/2$ , and  $l_2 = (5a^2 + 6ab + 5b^2)/16$ .

For the case of the normalised measure Eq. (240), we conclude that  $c_n^s = c_n^{s+1} \quad n, s = 0, 1, 2, \dots$  since its secondary normalised measure is equal to itself. Hence by denoting  $m_n = c_n^s \quad n, s = 0, 1, 2, \dots$  we can write Eq. (246) for this measure as

$$(m_2 - (m_1)^2) m_n = m_{n+2} - m_1 m_{n+1} - (m_2 - (m_1)^2) \sum_{j=0}^{n-1} m_j m_{n-j} \quad (250)$$

$n, s = 0, 1, 2, \dots$ . By direct calculation of the moments of Eq. (240), we find that  $m_0 = l_0$ ,  $m_1 = l_1$ ,  $m_2 = l_2$ , and hence by comparing Eq. (249) with Eq. (250) we conclude that  $m_n = l_n \quad n = 0, 1, 2, \dots$ . Thus using lemma (21) we conclude Eq. (240) under the assumptions Eq. (237) and (238). For Eq. (239), we note that Eq. (100) and Eq. (105) tell us  $\lim_{n \rightarrow \infty} \bar{\nu}_n(x) = \lim_{n \rightarrow \infty} \beta_n(d\mu_0) \bar{\mu}_n(x)$ . Hence from Eq. (238) and (240) we conclude Eq. (239).  $\square$

**Definition 23** We will call terminal spectral density  $J_T(\omega)$  the spectral density to which a sequence of partial spectral densities converge to weakly if such a limit exists:  $J_T(\omega) = \lim_{n \rightarrow \infty} J_n(\omega)$ .

We are now ready to state our fourth main theorem:

**Theorem 23** If for the particle or phonon mapping the spectral density  $J(\omega)$  belongs to the Szëgo class, the sequence of partial spectral densities converge to the Wigner semicircle distribution [37]

$$J_T(\omega) = \frac{\sqrt{\omega(\omega_{max} - \omega)}}{2}, \quad (251)$$

and the Rubin model spectral density [1]

$$J_T(\omega) = \frac{\omega \sqrt{(\omega_{max}^2 - \omega^2)}}{2}, \quad (252)$$

respectively.

*Proof* From Eq. (209) and theorem (22) we gather that if Eq. (237) and (238) are satisfied, then for the phonon case if we choose  $g_2 = 1$

$$J_T(\omega) = \frac{\sqrt{(\omega^2 - a)(b - \omega^2)}}{2}. \quad (253)$$

From Eq. (176) we have that  $a = 0$  and  $b = \omega_{max}^2$ . Now taking into account theorem (20), we get Eq. (252). Proceeding in a similar manner, we find Eq. (251).  $\square$

## 4 Examples

### 4.1 power law spectral densities with finite support

The the widely studied power law spectral densities is  $[10, 1]$

$$J(x) = 2\pi\alpha\omega_c^{1-s}x^s, \quad (254)$$

with domain  $[0, \omega_c]$  and  $s > -1$ . Let us start by calculating the sequence of partial spectral densities for the case of the particle mapping.

From Eq. (170) and (254) we have

$$M^0(x) = 2\alpha\omega_c^{1-s}x^s. \quad (255)$$

For simplicity, we will scale out the  $\omega_c$  dependency and show how to put it back again afterwards. Let us start by defining the weight function  $m_0^0(x) := \omega_c M^0(x\omega_c) = 2\alpha\omega_c^2 x^s$  with support interval  $[0, 1]$ . From lemma (12), we find that  $m_n^0(x) = M_n^0(x\omega_c)/\omega_c$   $n = 1, 2, 3, \dots$  where  $m_n^0(x)$  and  $M_n^0(x)$  are the sequence of beta normalised measures generated from  $m_0^0(x)$  and  $M^0(x)$  respectively. Now let us define the weight function

$$\tilde{m}_0^0(x) = x^s \quad (256)$$

with support interval  $[0, 1]$ . Given that this new measure is proportional to  $m_0^0(x)$ , from lemma (13) we conclude that it's sequence of beta normalised measures  $\tilde{m}_n^0(x)$   $n = 1, 2, 3, \dots$ , are equal. Hence we have  $M_n^0(x) = \omega_c \tilde{m}_n^0(x/\omega_c)$   $n = 1, 2, 3, \dots$ . Thus taking into account Eq. (170) and (221), setting  $g_2 = 1$  we conclude

$$J_n(\omega) = \pi M_n^0(\omega) = \omega_c \pi \tilde{m}_n^0(\omega/\omega_c) \quad n = 1, 2, 3, \dots \quad (257)$$

The real polynomials orthogonal to the weight function  $\tilde{m}_0^0(x)$  are  $P_n^s(x) := P_n^{(0,s)}(2x - 1)\sqrt{n+s+1}$   $n = 0, 1, 2, \dots$ ; which are normalised shifted counterparts of the *Jacobi polynomials*  $P_n^{(\alpha,\beta)}(x)$   $n = 0, 1, 2, \dots$ . The reducer for the case  $s \geq 0$  is given by theorem (25)

$$\varphi(d\tilde{m}^0; t) = 2 \left[ \ln \left( \frac{t}{1-t} \right) + s \int_0^1 x^{s-1} \ln \left| \frac{t-x}{t} \right| dx \right], \quad (258)$$

which has analytic solutions when a particular value of  $s$  is specified. For example, the first three in the sequence for the ohmic case ( $s = 1$ ) are

$$\tilde{m}_1^0(x) = \frac{x}{2(\pi^2 x^2 + [1 + x \ln(\frac{1-x}{x})]^2)}, \quad (259)$$

$$\tilde{m}_2^0(x) = \frac{x}{4\pi^2(2-3x)^2 x^2 + [1-6x + (4-6x)x \ln(\frac{1-x}{x})]^2}, \quad (260)$$

$$\tilde{m}_3^0(x) = \frac{6x}{36\pi^2 x^2(3-12x+10x^2)^2 + [30x-16 + (18-72x+60x^2)(1+x \ln(\frac{1-x}{x}))]^2}.$$

The chain coefficients are calculated in [18] to be

$$\alpha_n(0)(s) = \frac{\omega_c}{2} \left( 1 + \frac{s^2}{(s+2n)(2+s+2n)} \right) \quad n = 0, 1, 2, \dots, \quad (261)$$

$$\sqrt{\beta_{n+1}(0)}(s) = \frac{\omega_c(1+n)(1+s+n)}{(s+2+2n)(3+s+2n)} \sqrt{\frac{3+s+2n}{1+s+2n}} \quad n = 0, 1, 2, \dots, \quad (262)$$

$$(263)$$

where the  $(s)$  is to remind us of their  $s$  dependency. System environment coupling coefficient is [18]

$$\sqrt{\beta(0)} = \omega_c \sqrt{\frac{2\alpha}{s+1}}. \quad (264)$$

Now we will find the sequence of partial spectral densities for the case of the phonon mapping. From Eq. (175) and (254) we have

$$M^1(x) = 2\alpha\omega_c^{1-s}x^{s/2}, \quad (265)$$

with support  $[0, \omega_c^2]$ . Proceeding as in the particle mapping case and taking into account Eq. (209), we find

$$J_n(\omega) = \pi M_n^1(\omega^2) = \omega_c^2 \pi \tilde{m}_n^1(\omega^2/\omega_c^2) \quad n = 1, 2, 3, \dots, \quad (266)$$

where  $\tilde{m}_n^1(x)$   $n = 1, 2, 3, \dots$ , are the sequence of beta normalised measures generated from

$$\tilde{m}_0^1(x) = x^{s/2}, \quad (267)$$

with support  $[0, 1]$ . Let us denote  $\tilde{m}_0^1(x)$  and  $\tilde{m}_0^0(x)$  by  $\tilde{m}_{0s}^1(x)$  and  $\tilde{m}_{0s}^0(x)$  respectively to remind us of their  $s$  dependency. By comparing eq. (267) with eq. (256), we have that  $\tilde{m}_{0s}^1(x) = \tilde{m}_{0s/2}^0(x)$  for all  $s > -1$  and hence from Eq. (257) and (266) we see that for the Spin-Boson models, there is a simple relationship between the partial spectral densities of the particle and phonon mappings for different  $s$  values. For the same example as in the particle case ( $s = 1$ ), we need to evaluate  $m_n^0(x)$   $n = 1, 2, 3, \dots$ , for  $s = 1/2$ . The first one in the sequence is

$$\tilde{m}_1^1(x) = \frac{2\sqrt{x}}{3(\pi^2 x + (2 - 2\sqrt{x} \tanh^{-1}(\sqrt{x}))^2)}, \quad (268)$$

where  $\tanh^{-1}(x)$  is the inverse hyperbolic tangent function. We can readily calculate the chain coefficients from the particle example. By comparing the expression for the  $\alpha_n$  and  $\beta_n$  coefficients for the weight functions for the particle and phonon mappings, we find

$$\alpha_n(1)(s) = \omega_c \alpha_n(0)(s/2) \quad n = 0, 1, 2, \dots, \quad (269)$$

$$\sqrt{\beta_{n+1}(1)(s)} = \omega_c \sqrt{\beta_{n+1}(0)(s/2)} \quad n = 0, 1, 2, \dots, \quad (270)$$

and system environment coupling term to be

$$\sqrt{\beta(1)} = 2\omega_c \sqrt{\frac{\alpha\omega_c}{s+2}}. \quad (271)$$

For both the particle and phonon mappings, it is easy to verify that the chain coefficients and sequence of partial spectral densities will converge because Eq. (234) is satisfied in both cases as long as  $s < \infty$ . We also see that the sequence of partial spectral densities calculated in the above examples converge very rapidly to this limit after about the 3rd partial spectral density.

#### 4.2 The power law spectral densities with exponential cut off

The power law spectral densities with exponential cut off is [10, 1]

$$J(x) = 2\pi\alpha\omega_c^{1-s}x^s e^{-x/\omega_c}, \quad (272)$$

with domain  $[0, \infty)$  and  $s > -1$ . Let us start by calculating the sequence of partial spectral densities for the case of the particle mapping.

From Eq. (170) and (272) we have

$$M^0(x) = 2\alpha\omega_c^{1-s}x^s e^{-x/\omega_c}. \quad (273)$$

Let us define the measure  $m^0(x) := \omega_c M^0(x\omega_c) = 2\alpha\omega_c^2 x^s e^{-x}$  with support interval  $[0, \infty)$ . From lemma (12), we find that  $m_n^0(x) = M_n^0(x\omega_c)/\omega_c$   $n = 1, 2, 3, \dots$  where  $m_n^0(x)$  and  $M_n^0(x)$  are the sequence of beta normalised measures generated from  $m^0(x)$  and  $M^0(x)$  respectively. We will now define a 3rd measure by  $\tilde{m}^0(x) = x^s e^{-x}$ . We note that it is proportional to the measure  $m^0(x)$  and hence lemma (13) tells us that its sequence of beta normalised measures are equal. Thus we have the relation

$$M_n^0(x) = \omega_c \tilde{m}_n^0(x/\omega_c) \quad n = 1, 2, 3, \dots \quad (274)$$

The real polynomials orthogonal to the weight function  $\tilde{m}^0(x)$  are called the *associated Laguerre polynomials*  $L_n^s(x)$   $n = 0, 1, 2, \dots$ . Their normalised counterparts are  $P_n^s(x) := L_n^s(x) n!/\Gamma(n+s+1)$   $n = 0, 1, 2, \dots$ . The reducer in this case is given by theorem (25)

$$\varphi(d\tilde{m}^0; x) = 2 \int_0^{+\infty} (s-t)t^{s-1}e^{-t} \ln \left| \frac{t-x}{x} \right| dt, \quad (275)$$

which has analytic values when a particular value of  $s$  is specified. For example, if  $s$  is integer, we get

$$\varphi(d\tilde{m}^0; x) = 2 \left[ x^s e^{-x} Ex(x) - \sum_{k=0}^{s-1} (s-k-1)! x^k \right], \quad (276)$$

where  $Ex(x)$  is the *exponential integral* function[38].

From Eq. (221) followed by Eq. (274) we have

$$J_n(\omega) = \pi M_n^0(\omega) = \omega_c \pi \tilde{m}_n^0(\omega/\omega_c) \quad n = 1, 2, 3, \dots, \quad (277)$$

and Eq. (99) tells us

$$\tilde{m}_n^0(x) = \frac{x^s e^{-x}}{\left( P_{n-1}^s(x) \frac{\varphi(d\tilde{m}_n^0; x)}{2} - Q_{n-1}^s(x) \right)^2 + \pi^2 x^{2s} e^{-2x} P_{n-1}^s(x)^2} \quad n = 1, 2, 3, \dots \quad (278)$$

For example, the first two in the sequence for the ohmic case ( $s = 1$ ) are

$$\tilde{m}_1^0(x) = \frac{x e^x}{e^{2x} + \pi^2 x^2 - 2x Ex(x) e^x + x^2 Ex(x)^2}, \quad (279)$$

$$\tilde{m}_2^0(x) = \frac{2x e^x}{e^{2x}(1-x)^2 + \pi^2 x^2(x-2)^2 - 2x(2-3x+x^2)Ex(x)e^x + x^2(x-2)^2 Ex(x)^2}. \quad (280)$$

We also have analytic expressions for the chain coefficients. From [18], we have that the chain coefficients are

$$\sqrt{\beta_{n+1}(0)} = \omega_c \sqrt{(n+1)(n+s+1)} \quad n = 0, 1, 2, \dots, \quad (281)$$

$$\alpha_n(0) = \omega_c(2n+1+s) \quad n = 0, 1, 2, \dots, \quad (282)$$

with the system-environment coupling coefficient given by

$$\sqrt{\beta_0(0)} = \omega_c \sqrt{2\alpha\Gamma(s+1)}. \quad (283)$$

Similarly, we can calculate the partial spectral densities and chain coefficients for the phonon mapping case.

Because the support interval is infinite, the Spin-Boson model with exponential cut off does not belong to the Szëgo class for either the particle mapping nor the phonon mapping as can be easily verified from Eq. (234). This is reflected in the example above as the sequence of partial spectral densities do not converge<sup>8</sup>.

*Remark 8* We note that for spectral densities for which the corresponding orthogonal polynomials are unknown analytically, we can easily calculate their coefficients using very stable numerical algorithms. See [19] or [18] and references herein for more details.

---

<sup>8</sup> However, we do note that the ratio  $\alpha_n(q)/\sqrt{\beta_{n+1}(q)}$  for  $q = 0$  and  $q = 1$  does converge. This suggests that there is a universal asymptotic expansion for large  $n$  for the  $n$ th partial spectral density.

## 5 Summary and conclusion

By developing the method of [18,19], we have established a general formalism for mapping an open quantum system of arbitrary spectral density of the form Eq. (119) onto chain representations. The different versions of chain mappings are generated by choosing particular values of 4 real constants. This has also provided a very general connection between the theory of open quantum systems and Jacobi operator theory as the semi-infinite chains can be written in terms of Jacobi matrices as can be seen in corollary (6). There has been a wealth of research into the properties of Jacobi operator theory [25], and hence this opens up the theorems of this field to the possibility of being applied to the theory of open quantum systems. Likewise, the new theorem regarding Jacobi matrices (15) developed here, could turn out to be useful in the field of Jacobi operator theory.

There were two previously known exact chain mappings; the one of [18] which is the same as the particle mapping defined here (definition 17), and the mapping by [21]. We point out that the phonon mapping derived in this article (18) has a wider range of validity (remark 6) than the mapping of [21] and prove that they are formally equivalent in the range of validity of [21]; see theorem (18).

The concept of embedding degrees of freedom into the system has been around for some time [24,21], however, we see that in chain representations, there is a natural way of shifting the system-environment boundary, that is to say, there is a natural and systematic way of embedding degrees of freedom into the system one by one (or all in one go). To solve quantitatively this problem, we have to first embark on finding the solution to an old problem in mathematics; an analytical solution to the sequence of secondary measures in terms of the initial measure, its associated orthogonal polynomials and reducer; see theorem (12). Not only does this provide a means to find analytical expressions for the sequence of spectral densities corresponding to the new system-environment interaction after embedding environmental degrees of freedom into the system for the particle and phonon mappings in the gapless spectral densities case (theorem (19) and corollary (7) respectively), but it provides physical meaning to this abstract mathematical construct.

Using convergence theorems of Szegő and deriving the fixed point in the sequence of secondary measures; we have combined these results to obtain a convergence theorem of the sequence of partial spectral densities for the particle and phonon cases, theorem (23) (or equivalently, the sequence of secondary measures, theorem (22)). What is more, because the criterion for convergence (definition 21) is solely in terms of the initial spectral density once the desired chain mapping is chosen, the convergence criterion is readily applicable to a particular problem. Furthermore, we see that any unbounded spectral density will not satisfy this criterion. This is reflected in the sequence generated in the examples section for the case of the family of power-law spectral densities with exponential cut off as the sequence does not converge, section 4.2.

We give two examples where we can find explicit analytical expressions for the chain coefficients and the sequence of partial spectral densities. These are the family of spectral densities used in the Spin-Boson model, which have spectral densities of the form  $x^s$  with finite support  $I = [0, \omega_c]$  and  $x^s e^{x/\omega_c}$  with semi-infinite support  $I = [0, +\infty)$ , where  $s > -1$ . Furthermore, we show how the partial spectral densities of the mapping for both phonon and particle cases are related for different families of the mapping as demonstrated by the identity  $\tilde{m}_{0s}^1(x) = \tilde{m}_{0s/2}^0(x)$  and Eq. (257) and (272).

We note that when this convergence of the embeddings is achieved (i.e. inequality (234) is satisfied), the part of the chain corresponding to the new environment has a very universal property: all its couplings and frequencies become constant. This is to say, they are translationally invariant. This suggests a universal way of simulating the environment as all the characteristic features of the environment are now embedded into the system, as discussed for the mapping of [18] in [22]. What is not so clear however, is what is the most effective chain mapping for simulating the environment. The general formalism of chain mapping for open quantum systems developed here, paves the way to answering these questions.

## 6 Appendix

### 6.1 Alternative proof for the sequence of partial spectral densities for the phonon mapping

We note that by applying the same line of reasoning of the proof for theorem (19) to the phonon mapping Hamiltonian Eq. (173), we can easily provide an alternative proof for corollary (7). This has the advantage of being an independent derivation of the results of [21], but has the downside of not illustrating the connections between this paper and their results.

### 6.2 Methods for calculating the reducer

**Theorem 24** *If for a measure  $d\mu(x) = \bar{\mu}(x)dx$ ,  $\bar{\mu}(x)$  satisfies a Lipschitz condition over its support interval  $[a, b]$ , then*

$$\varphi(d\mu; x) = 2\bar{\mu}(x) \ln \left( \frac{x-a}{b-x} \right) - 2 \int_a^b \frac{\bar{\mu}(t) - \bar{\mu}(x)}{t-x} dt. \quad (284)$$

*Proof* From definitions (11) and (7) we get

$$\varphi(d\mu; x) = \lim_{\epsilon \rightarrow 0^+} 2 \int_a^b \frac{(x-t)\bar{\mu}(t)dt}{(x-t)^2 + \epsilon^2}. \quad (285)$$

Writing this as

$$\varphi(d\mu; x) = \lim_{\epsilon \rightarrow 0^+} 2 \int_a^b \frac{(x-t)\bar{\mu}(x)}{(x-t)^2 + \epsilon^2} dt + \lim_{\epsilon \rightarrow 0^+} 2 \int_a^b \frac{(x-t)(\bar{\mu}(t) - \bar{\mu}(x))}{(x-t)^2 + \epsilon^2} dt \quad (286)$$

$$= \lim_{\epsilon \rightarrow 0^+} 2 \int_a^b \frac{(x-t)\bar{\mu}(x)}{(x-t)^2 + \epsilon^2} dt - 2 \int_a^b \frac{\bar{\mu}(t) - \bar{\mu}(x)}{t-x} dt \quad (287)$$

$$- \lim_{\epsilon \rightarrow 0^+} \int_a^b \left( \frac{2\epsilon^2}{(x-t)^2 + \epsilon^2} \right) \frac{\bar{\mu}(t) - \bar{\mu}(x)}{x-t} dt. \quad (288)$$

1) The first integral in line (287) reduces to

$$\lim_{\epsilon \rightarrow 0^+} 2 \int_a^b \frac{(x-t)\bar{\mu}(x)}{(x-t)^2 + \epsilon^2} dt = \lim_{\epsilon \rightarrow 0^+} \bar{\mu}(x) [\ln((a-x)^2 + \epsilon^2) - \ln((b-x)^2 + \epsilon^2)] \quad (289)$$

$$= 2\bar{\mu}(x) \ln \left( \frac{x-a}{b-x} \right). \quad (290)$$



- 2) Now imposing the Lipschitz condition on  $\bar{\mu}(x)$ :  $|\bar{\mu}(x) - \bar{\mu}(t)| \leq K|t - x|$  for some  $K$  over interval  $[a, b]$ , the absolute value of the expression on line (288) reduces to

$$\lim_{\epsilon \rightarrow 0^+} \int_a^b \left( \frac{2\epsilon^2}{(x-t)^2 + \epsilon^2} \right) \frac{|\bar{\mu}(t) - \bar{\mu}(x)|}{|t-x|} dt \quad (291)$$

$$\leq \lim_{\epsilon \rightarrow 0^+} \int_a^b \frac{2K\epsilon^2}{(x-t)^2 + \epsilon^2} dt \quad (292)$$

$$= \lim_{\epsilon \rightarrow 0^+} 2K\epsilon \left[ \arctan \left( \frac{b-x}{\epsilon} \right) - \arctan \left( \frac{a-x}{\epsilon} \right) \right] \quad (293)$$

$$= 0. \quad (294)$$

Hence expression on line (288) vanishes.

□

**Lemma 11** *If  $f(x)$  possesses a bounded continuous first derivative on its domain, then it also satisfies a Lipschitz condition on its domain.*

*Proof* See [39].

**Theorem 25** *If for a measure  $d\mu(x) = \bar{\mu}(x)dx$ ,  $\bar{\mu}(x)$  possesses a bounded continuous first derivative on its support interval  $I$  and  $\bar{\mu}(x)$  can be evaluated on the limits  $a, b$ , then*

$$\varphi(d\mu; x) = 2 \left[ \bar{\mu}(a) \ln \left| \frac{x-a}{x} \right| + \bar{\mu}(b) \ln \left| \frac{x}{b-x} \right| + \int_a^b \bar{\mu}'(t) \ln \left| \frac{t-x}{x} \right| dt \right], \quad (295)$$

where  $\bar{\mu}'(t)$  is the first derivative of  $\bar{\mu}(t)$ .

*Proof* Follows from integrating Eq. (284) by parts and applying lemma (11). □

### 6.3 Scaling properties of the sequence of beta normalised measures

**Lemma 12** *Suppose we have two measures  $d\nu^1(x) = \bar{\nu}^1(x)dx$  and  $d\nu^2(x) = \bar{\nu}^2(x)dx$  with support intervals  $I^1, I^2$  bounded by  $\lambda a, \lambda b$  and  $a, b$  respectively. If they are related by*

$$\bar{\nu}^1(x) = \frac{\bar{\nu}^2(x/\lambda)}{\lambda}, \quad \lambda > 0, \quad (296)$$

then their sequence of beta normalised measures have the relation

$$\bar{\nu}_n^1(x) = \lambda \bar{\nu}_n^2(x/\lambda) \quad n = 1, 2, 3, \dots \quad (297)$$

*Proof* Using the definition of inner product, definition (2), and relation eq. (296), we find

$$\langle f, g \rangle_{\bar{\nu}^2} = \int_a^b f(\lambda t) g(\lambda t) d\nu^1(t). \quad (298)$$

Hence we conclude

$$P_n(d\nu^1; x) = P_n(d\nu^2; x/\lambda) \quad n = 0, 1, 2, \dots \quad (299)$$

Using this relation and definition (6), we find

$$Q_n(d\nu^1; x) = \frac{Q_n(d\nu^2; x/\lambda)}{\lambda} \quad n = 0, 1, 2, \dots \quad (300)$$

Similarly, we have from definition (11)

$$\varphi(d\nu^1; x) = \frac{\varphi(d\nu^1; x/\lambda)}{\lambda}. \quad (301)$$

Finally, substituting Eq. (299), (300), and (301) into definition (13) we arrive at Eq. (297).  $\square$

**Lemma 13** *The sequence of beta normalised measures generated from a measure  $d\nu(x) = \bar{\nu}(x)dx$  are invariant under the mapping  $d\nu(x) \rightarrow \lambda d\nu(x)$ ,  $\lambda > 0$  while keeping the support interval  $I$  unchanged.*

*Proof* Follows with a similar line of reasoning as for lemma (12).  $\square$

*Acknowledgements* We acknowledge Sebastian Karl Egger for discussions regarding mathematical technicalities, Nicolas Neumann for pointing out typos and Ramil Nigmatullin for help with latex formatting. This work was supported by the EPSRC CDT on Controlled Quantum Dynamics, the EU STREP project CORNER and the EU Integrating project Q-ESSENCE as well as the Alexander von Humboldt Foundation.

## References

1. Weiss, U.: *Quantum Dissipative Systems*, World Scientific, Singapore, 2001
2. Breuer, H.P. and Petruccione, F.: *The Theory of Open Quantum Systems*, Oxford University Press, 2002
3. Rivas A. and Huelga, S.F.: *Open Quantum Systems. An Introduction*, Springer Briefs in Physics, Springer, 2011, ISBN: 978-3-642-23353-1
4. Engel, G.S., Calhoun, T.R., Read, E.L., Ahn, T.K., Caronal, T.M., Cheng, Y.C., Blankenship, R.E. and Fleming, G.R.: Evidence for wavelike energy transfer through quantum coherence in photosynthetic systems, *Nature* **446**, 782-786 (2007)
5. Mohseni, M., Rebentrost, P., Lloyd, S. and Aspuru-Guzik, A.: Environment-assisted quantum walks in photosynthetic energy transfer, *J. Chem. Phys.* **129**, 174106 (2008)
6. Plenio, M.B. and Huelga, S.F.: Dephasing-assisted transport: quantum networks and biomolecules, *New J. Phys.* **10**, 113019 (2008)
7. Caruso, F., Chin, A.W., Datta, A., Huelga, S.F. and Plenio, M.B.: Highly efficient energy excitation transfer in light-harvesting complexes: The fundamental role of noise-assisted transport, *J. Chem. Phys.* **131**, 105106 (2009)
8. Proceedings of the 22nd Solvay Conference on Chemistry *Quantum Effects in Chemistry and Biology*, *Procedia Chemistry* **3**, 1 - 366 (2011)
9. Fleming, G.R., Huelga, S.F. and Plenio, M.B.: Focus on quantum effects and noise in biomolecules, *New J. Phys.* **13** 115002 (2011)
10. Leggett, A.J., Chakravarty, S., Dorsey, A.T., Fisher, M.P.A., Garg, A. and Zwerger, W.: Dynamics of the dissipative two-state system, *Rev. Mod. Phys.* **59**, 1-85 (1987)
11. Rivas, A., Huelga, S.F. and Plenio, M.B.: Entanglement and Non-Markovianity of Quantum Evolutions, *Phys. Rev. Lett.* **105**, 050403 (2010)

12. Laine, E.M., Piilo, J. and Breuer, H.P.: Measure for the non-Markovianity of quantum processes, *Phys. Rev. A*, **81**, 062115 (2010)
13. Wolf, M.M., Eisert, J., Cubitt, T.S. and Cirac, J.I.: Assessing non-Markovian dynamics, *Phys. Rev. Lett.* **101**, 150402 (2008)
14. Silbey, R. and Munn, R.W.: General theory of electronic transport in molecular crystals. I. Local linear electron-phonon coupling. *J. Chem. Phys.* **72**, 27632773 (1980)
15. Makri, N.: Numerical path integral techniques for long-time quantum dynamics of dissipative systems, *J. Math. Phys.* **36**, 2430 (1995)  
Thorwart M., Eckel, J., Reina, J.H., Nalbach, P., Weiss, S.: Enhanced quantum entanglement in the non-Markovian dynamics of biomolecular excitons, *Chem. Phys. Lett.* **478**, 234 (2009)
16. Ishizaki, A., Tanimura, Y.: Quantum Dynamics of System Strongly Coupled to Low-Temperature Colored Noise Bath: Reduced Hierarchy Equations Approach, *J. Phys. Soc. Jap.* **12**, 31313134 (2005)  
Ishizaki, A., Fleming, G.R.: Unified treatment of quantum coherent and incoherent hopping dynamics in electronic energy transfer: Reduced hierarchy equation approach, *J. Chem. Phys.* **130**, 234111 (2009)
17. Roden, J., Eisfeld, A., Wolff, W., Strunz, W. T.: Influence of Complex Exciton-Phonon Coupling on Optical Absorption and Energy Transfer of Quantum Aggregates, *Phys. Rev. Lett.* **103**, 058301 (2009)
18. Chin, A.W., Rivas, A., Huelga, S.F. and Plenio, M.B.: Exact mapping between system-reservoir quantum models and semi-infinite discrete chains using orthogonal polynomials, *J Math Phys* **51**, 092109 (2010)
19. Prior, J., Chin, A.W., Huelga, S.F., Plenio, M.B.: Efficient Simulation of Strong System-Environment Interactions, *Phys. Rev. Lett.* **105**, 050404, (2010)
20. Vojta, M., Tong, N.H., Bulla, R.: Quantum Phase Transitions in the Sub-Ohmic Spin-Boson Model: Failure of the Quantum-Classical Mapping, *Phys. Rev. Lett.* **94**, 070604 (2005)  
Bulla, R., Costi, T. and Pruschke, T.: Numerical renormalization group method for quantum impurity systems, *Rev. Mod. Phys.* **80**, 395 (2008)
21. Martinazzo, R., Vacchini, B., Hughes, K.H. and Burghardt, I.: Universal Markovian reduction of brownian particle dynamics, *J. Chem. Phys.* **134**, 011101, (2011)
22. Chin, A.W., Huelga, S.F. and Plenio, M.B.: *Chapter 7: Chain representations of open quantum systems and their numerical simulation with time-adaptive density matrix renormalisation group methods*, To appear in *Semiconductors and Semimetals*, Volume 85, Elsevier, London, (2012)
23. Martinazzo, R., Hughes, K.H. and Burghardt, I.: Unraveling a Brownian particle's memory with effective mode chains, *Phys. Rev. E* **84**, 030102 (2011)
24. Imamoglu, A.: Stochastic wave-function approach to non-Markovian systems, *Phys. Rev. A* **50**, 3650-3653 (1994)  
Garraway, B.M.: Nonperturbative decay of an atomic system in a cavity, *Phys. Rev. A* **55**, 2290-2303 (1997)  
Breuer, H.-P.: Genuine quantum trajectories for non-Markovian processes, *Phys. Rev. A* **70**, 012106 (2004)
25. Teschl, G.: *Jacobi Operators and Completely Integrable Nonlinear Lattices*, Mathematical Surveys and Monographs, Volume 72, Amer. Math. Soc., Providence (2000)
26. John, S.: Strong localization of photons in certain disordered dielectric superlattices, *Phys. Rev. Lett.* **58**, 2486 (1987)  
Yablonovitch, E.: Inhibited Spontaneous Emission in Solid-State Physics and Electronics, *Phys. Rev. Lett.* **58**, 2059 (1987)
27. Gautschi, W.: *Orthogonal Polynomials, Computation and Approximation*, (Numerical Mathematics and Scientific Computation), Oxford Science Publications, ISBN 0-19-850672-4
28. Berg, C.: *Annales de la Faculté des Sciences de Toulouse, Sér 6 Vol. S5* (1996), p.932

29. Shermann, J.: On the numerators of the convergents of the Stieltjes continued fractions, Trans.Amer. Math.Soc. **35**, 64-87 (1933)
30. Groux, R.: Sur une mesure rendant orthogonaux les polynomes secondaires, C.R Acad.Sci. Paris, Ser.I. **345**, 373-376 (2007)
31. Backer, G.A., and Graves-Morris, P.: *Pade approximants*, Cambridge University Press, (1965)
32. Buchwalter, H., *Theorie Spectrale*, Cours de DEA universite Claude Bernard Lyon, Chapter 1, (1983)
33. Caldeira, A. and Leggett, A.: Quantum Tunnelling in a Dissipative System, Annals of Physics **149**, 374-456 (1983)
34. Blaizot, J.-P. and Ripka, G.: *Quantum Theory of Finite Systems*. MIT Press (1985)
35. Leggett, A.J.: Quantum tunneling in the presence of an arbitrary linear dissipation mechanism, Phy. Rev. B. **30**, 12081218 (1984)  
Garg, A., Onuchic, J.N. and Ambegaokar, V.: Effect of friction on electron transfer in biomolecules, J. Chem. Phys. **83**, 4491 (1985)
36. Szegő, G.: *Orthogonal Polynomials*, American Mathematical Society, Providence, Rhode Island (1975). See chapter 12
37. Arnold, L.: On Wigner's Semicircle Law for the Eigenvalues of Random Matrices, Journal of Probability theory and related fields, p191-198, Vol 19, issue 3. Springer (1971)
38. Abramowitz, M. and Stegun, I.A.: *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, New York: Dover. ISBN 0-486-61272-4
39. Adams, R.A. and Fournier, J.F.: *Sobolev Spaces*, Volume 140, Second Edition, Elsevier Science Ltd (2003), ISBN: 0-12-044143-8